DOE Bioenergy Technologies Office (BETO) 2019 Project Peer Review

2.1.0.100
Biochemical Platform Analysis

Biochemical Conversion

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Goal Statement

Objective

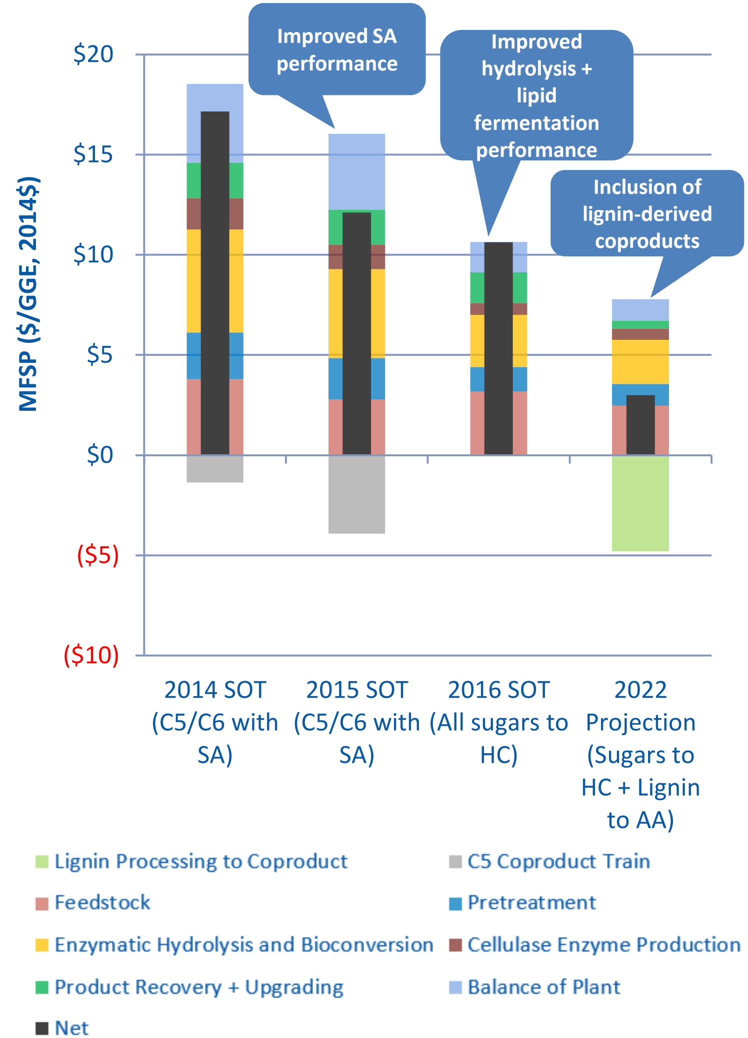
- Provide **process design and economic analysis support** for the biochemical conversion platform, to **guide R&D priorities towards economic viability**
    - Translate demonstrated/proposed research advances into economics (quantified as $/gal ($/GGE) selling price)

Outcomes

- Benchmark process models and economic analysis tools – used to:
    - Assess cost-competitiveness and **establish process/cost targets** for biofuel production pathways
    - **Track progress** towards goals through state of technology (SOT) updates
    - Provide input to **prioritize research**: identify impact of key variables and design alternatives on overall economics
    - **Disseminate** rigorous, objective modeling and analysis work in a transparent way (the "design report" process)

Relevance

- This project **directly supports the BETO Program** by providing "bottom-up" TEA to show R&D needs for achieving "top-down" BETO cost goals
    - *Guide R&D towards economic viability, eventual adoption of biofuels into U.S. market*



Example of the use of TEA to track historical progress towards goals for hydrocarbon fuels via prior lipid fermentation pathways

Quad Chart Overview

Timeline

- Start date: Oct 1, 2016 (current 3-year cycle)
- End date: Sept 30, 2019 (current 3-year cycle)
- Percent complete: 83% (year 3/Q2 of cycle)

Budget

	Total Costs Pre FY17**	FY 17 Costs	FY 18 Costs	Total Planned Funding (FY 19-Project End Date)
DOE Funded	NA (3-year cycle starts FY17)	$650k	$500k	$500k (FY19)
Project Cost Share*	NA	NA	NA	NA

- **Partners:** No partners with shared funding (but collaborate frequently with other modeling/analysis projects at INL, ANL, PNNL; also provide TEA support under separate funding for consortia including FCIC, ChemCatBio, Separations Consortium, Agile)

Barriers addressed

- ADO-A: Process Integration
  - *TEA models tie all R&D operations together*
- Ct-D: Advanced Bioprocess Development
  - *Highlight cost drivers and priorities/tradeoffs between titers, rates, yields, bioreactor operation*
- At-E: Quantification of Economic, Environmental, and Other Benefits and Costs
  - *Perform cost/benefit analyses, help define value proposition*

Objective

Conduct process modeling, TEA, and sustainability assessment to support Biochemical Platform R&D activities, relating key process parameters with overall economics. Establish process targets required to meet $2.5/GGE cost targets, and track progress towards those targets via SOT benchmarking.

End of Project Goal

Over current 3-year cycle, this project will assist the platform in down-selecting to the pathways for 2030 demo R&D focus, publish a new design report, and re-benchmark progress based on FY19 SOT performance and remaining gaps. Final year 3 goal: report on benchmarking progress based on SOT performance relative to prior projections, to validate efforts are on track for 2022 interim demos. Highlight key remaining gaps and TEA priorities.

Project Overview

- Long NREL history of rigorous process modeling
  - Set objective, transparent technology benchmarks
  - Quantify economic impact of funded R&D improvements relative to benchmarks
  - Evaluate sensitivities to inputs, uncertainties
  - "Basic engineering" and process optimization
- Phased Approach:
  - Develop baseline models with best available data
  - Validate and conduct peer review modeling assumptions, publish "design reports"
  - Iterate with researchers and external stakeholders, refine models with new data
- Types of Analysis:
  - Technoeconomic analysis (TEA)
  - Life-cycle analysis (LCA)/sustainability indicators
- Technology Focus:
  - 2001–2012: cellulosic ethanol
  - 2013+: hydrocarbon biofuels, bioproducts

Approach – Technical

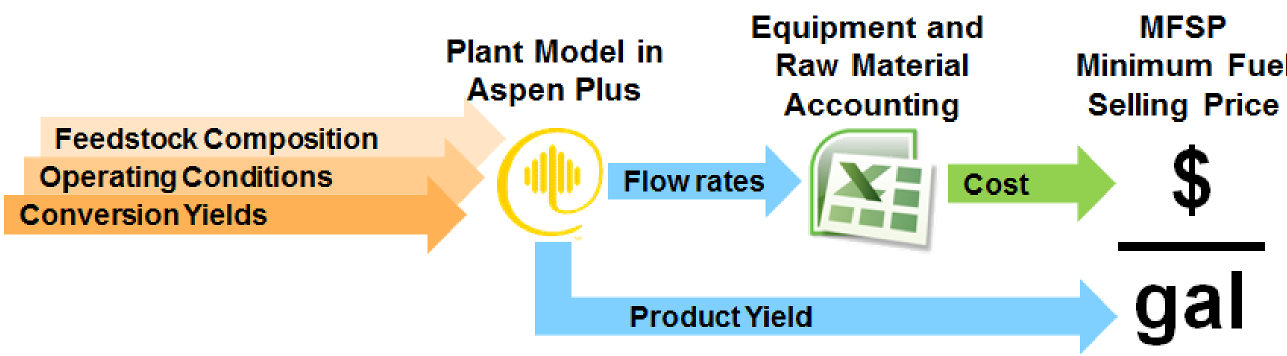
- Aspen Plus modeling for rigorous M&E balances
- Discounted cash-flow calculations determine minimum fuel selling price (MFSP) at fixed IRR
- Credibility of analysis supported by vendor cost estimates, thorough vetting with industry and research stakeholders

Critical Success Factors:

- Critical to **maintain credible engineering analyses** that are transparent and unbiased—work with engineering subcontractors to reduce uncertainty, subject design reports to thorough external peer review
- Provide accurate sensitivity analyses to **prioritize R&D, maximize efficiency of research funds**
- Be **open to new ideas,** alternative process concepts – no "single path" definitively better than others in achieving aggressive $2.5/GGE targets

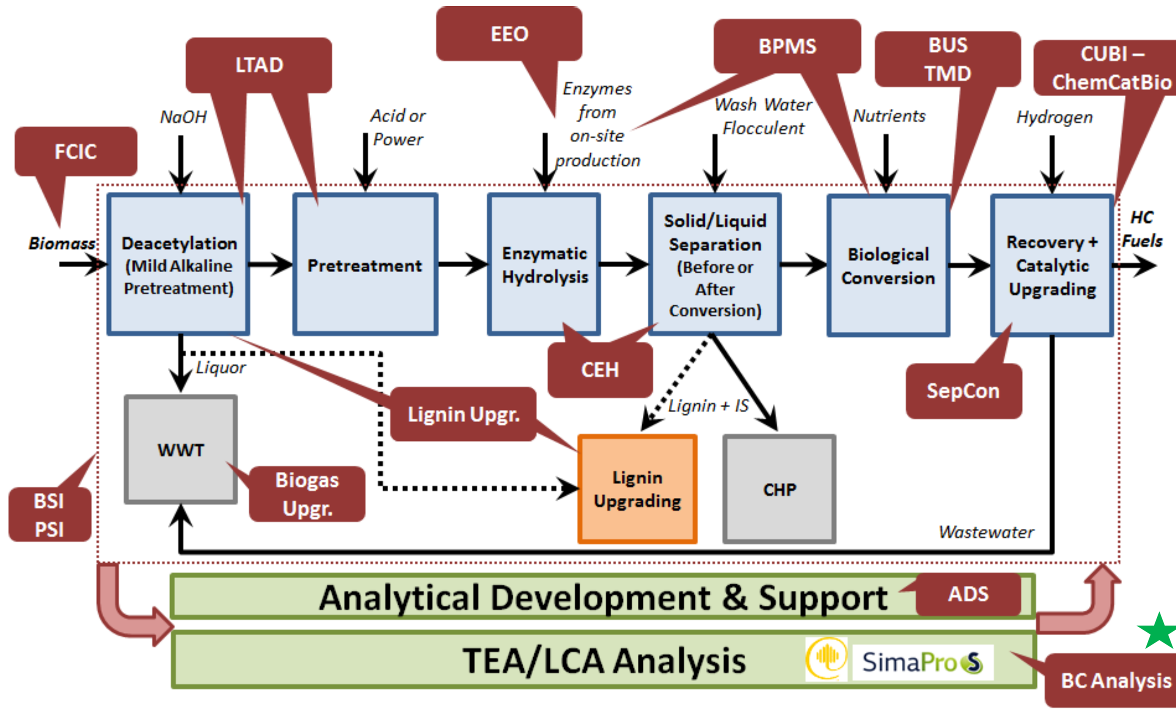
Challenges:

- **Models becoming increasingly complex**; challenges in setting design/cost parameters, extrapolating to nth-plant commercial scale
- More difficult to develop **representative models for new/novel low-TRL technologies** that are not yet well-understood for current performance or future best-case potential



Approach – Management

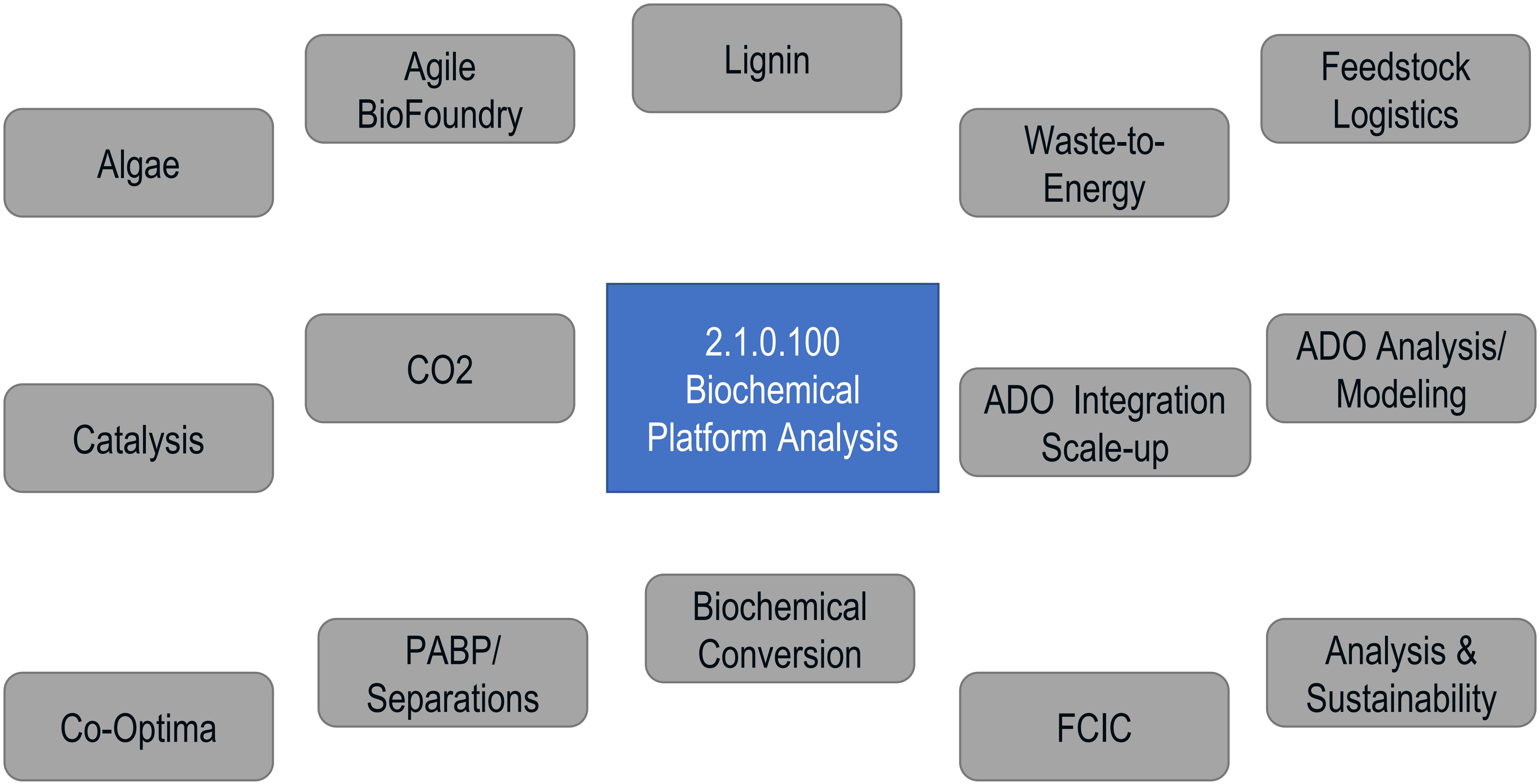
- Project management tracked using milestones
- **Activities are highly integrated with research efforts, assist in go/no-go decisions for R&D**
  - Example—FY18 go/no-go milestone to support down-select decision for pathways of focus in 2018 design report update



Project Milestones/Activities	FY17				FY18				FY19 (planned)			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
R&D/Platform Support												
TEA analysis for out-year target projections supporting $2.5/GGE	▼				▼	⬣	▼	▲				
SOT benchmarking				▲					▲			▲
Lignin coproduct modeling		▼								▼	▼	
Biogas upgrading TEA											▼	
Catalytic conversion pathways analysis		▲										
Design/Engineering Analysis/TEA Refinement												
Cost of aeration TEA/optimization			▼									
Updated sugar model	▼											
Cost/optimization for separations			▼									

▲ = Milestone, ▼ = Quarterly progress measure, ⬣ = Go/no-go decision

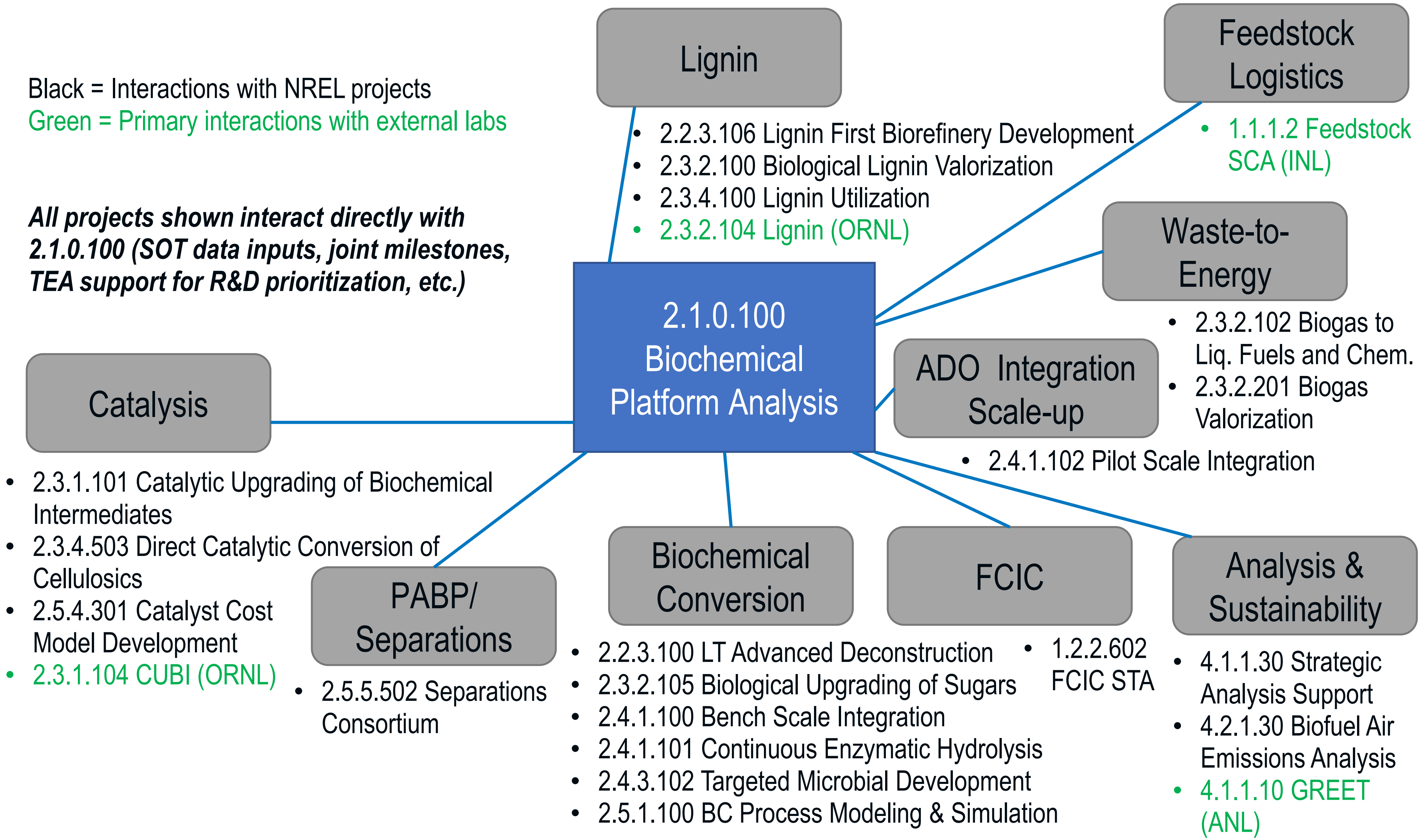
Approach – Management: Tie-Ins with Other Projects



Approach – Management: Tie-Ins with Other Projects

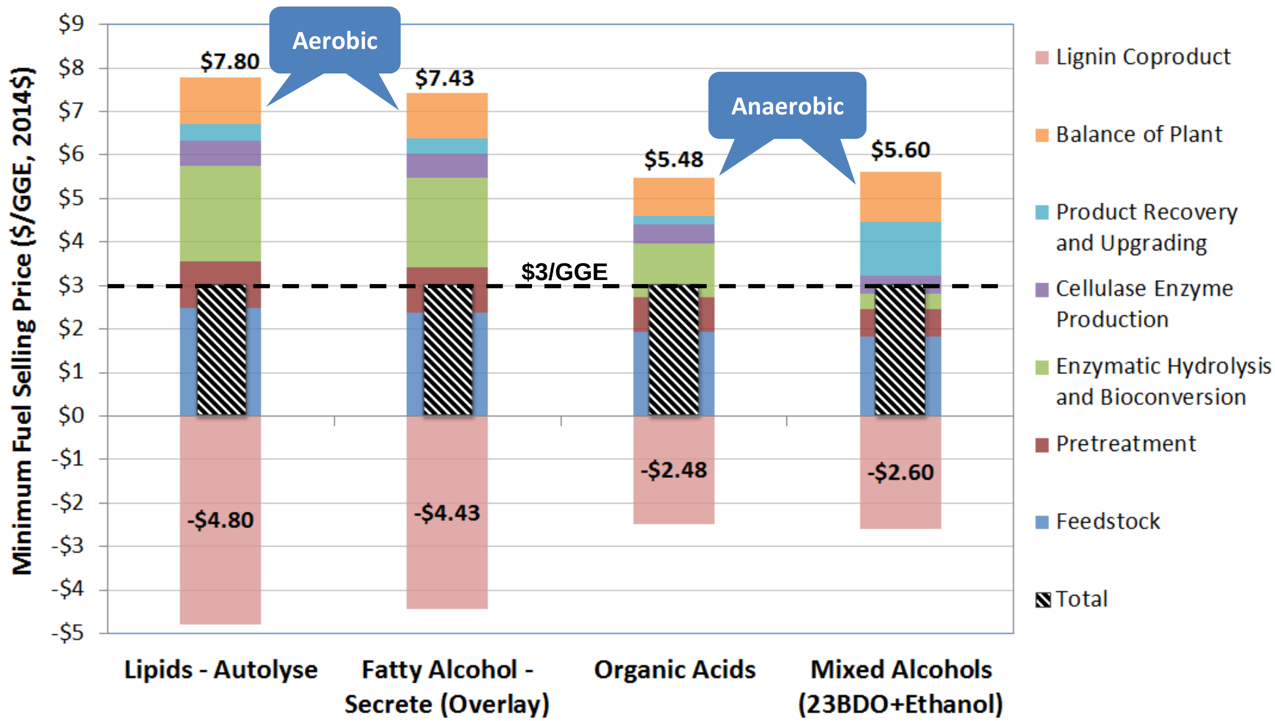
Black = Interactions with NREL projects
Green = Primary interactions with external labs

All projects shown interact directly with 2.1.0.100 (SOT data inputs, joint milestones, TEA support for R&D prioritization, etc.)



Technical Accomplishments/Progress/Results: *Down-Selection of Pathway Options to Support $2.5/GGE*

- Prior NREL work focused on four bioconversion options (2 aerobic, 2 anaerobic)
- **FY18 Q2 go/no-go: assist the Platform in down-selecting pathways** for design report
- Recommendation to **de-emphasize aerobic options** (lipids, fatty alcohols) to **focus more on anaerobic** (acids, BDO) per prior TEA work

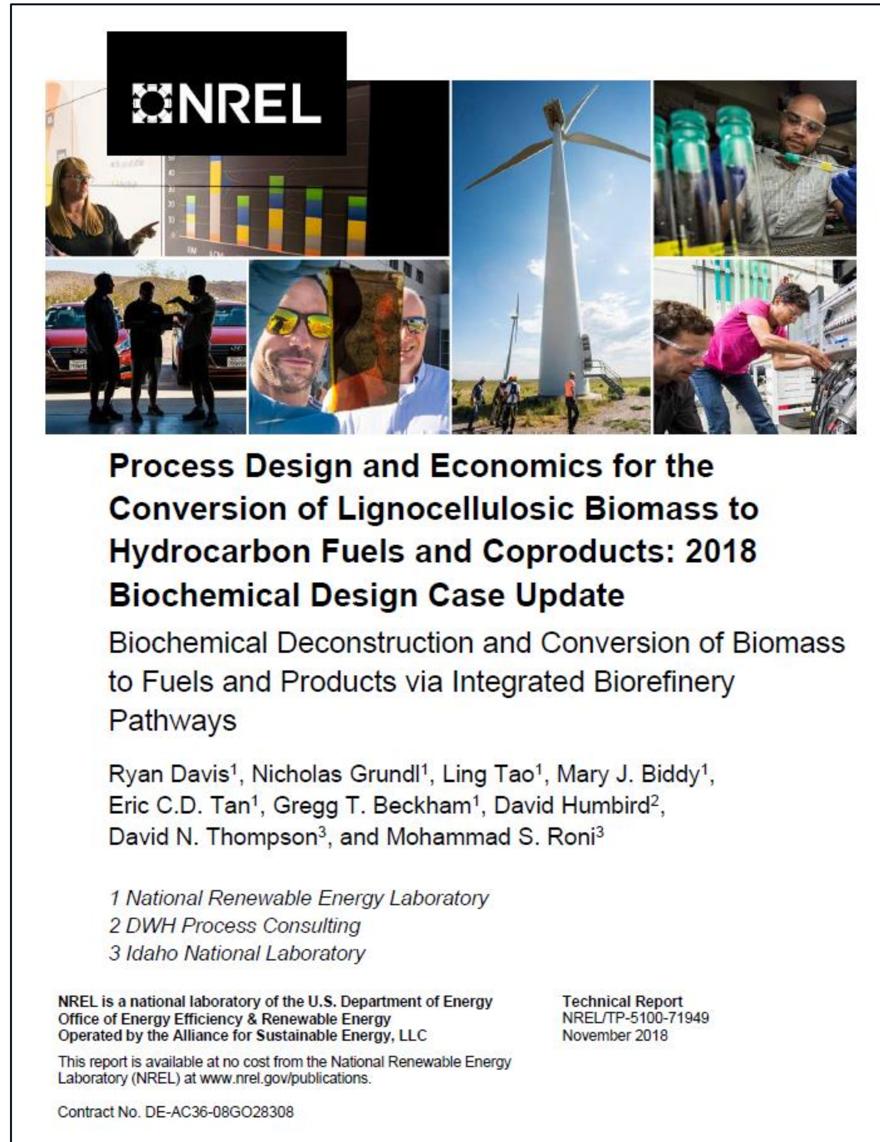


- Aerobic pathways = lower yields at higher costs, more burdens on coproducts for achieving MFSP targets
- Further challenges in TRL levels (fatty alcohols), product recovery costs (lipids)
- ***Not* a universal decision** against aerobic in all cases

Metric	Lipids	Fatty Alcohols	Organic Acids	BDO + EtOH
MFSP ($/GGE, 2014$) — Prior to coproducts	$7.80	$7.43	$5.48	$5.60
C efficiency (biomass to fuel)	20%	21%	25%	27%
Fuel yield (GGE/ton)	34.2	35.7	43.5	46.5
TCI ($MM) — Prior to coproducts	$640	$628	$520	$527
Carbon efficiency through lignin-to-coproduct train required to achieve $3/GGE	59%	56%	40%	46%

Technical Accomplishments/Progress/Results: *2018 Design Report Update*

- **First major update providing public documentation** of latest NREL R&D strategies/vision for biochemical (fermentative) process since 2013 report
- Relative to 2013 report (original framework focused on near-term $5/GGE case by 2017), 2018 report focuses on **longer-term strategies to achieving <$2.5/GGE MFSP goals by 2030**
- Bottom-up TEA modeling to establish technical targets for meeting top-down cost goals
- Transparent documentation of all inputs/assumptions (99 pages excluding appendices)
- **Vetted across 12 external reviewers** (experts from industry, research, academia) prior to publishing final draft


NREL

Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels and Coproducts: 2018 Biochemical Design Case Update

Biochemical Deconstruction and Conversion of Biomass to Fuels and Products via Integrated Biorefinery Pathways

Ryan Davis[1], Nicholas Grundl[1], Ling Tao[1], Mary J. Biddy[1], Eric C.D. Tan[1], Gregg T. Beckham[1], David Humbird[2], David N. Thompson[3], and Mohammad S. Roni[3]

1 National Renewable Energy Laboratory
2 DWH Process Consulting
3 Idaho National Laboratory

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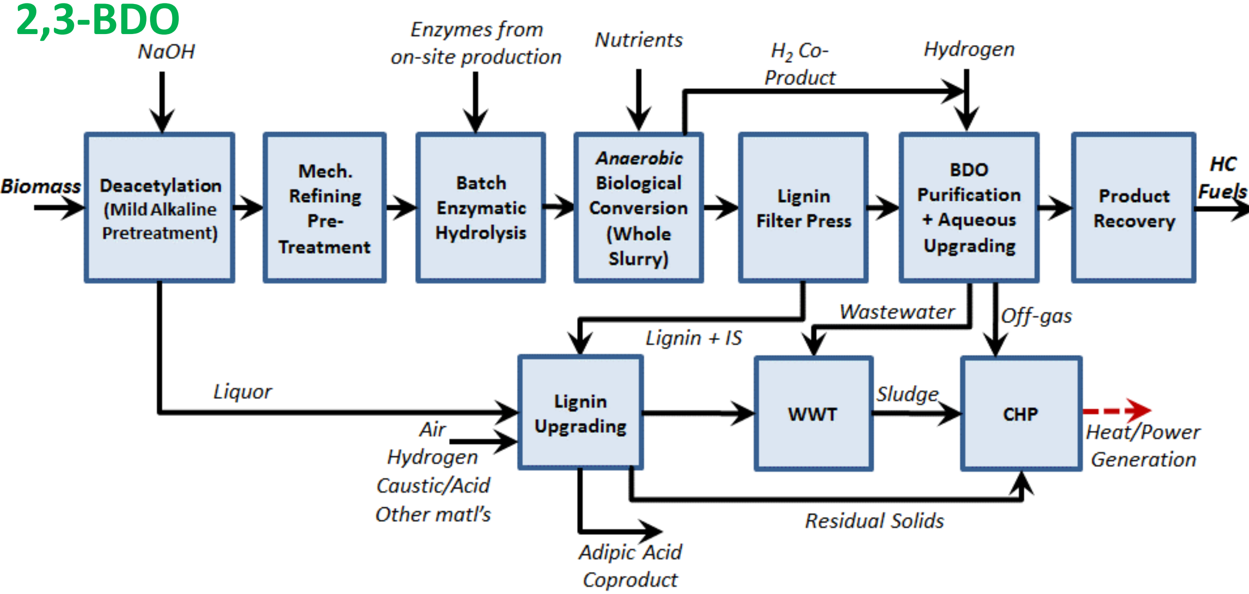
Contract No. DE-AC36-08GO28308

Technical Report
NREL/TP-5100-71949
November 2018

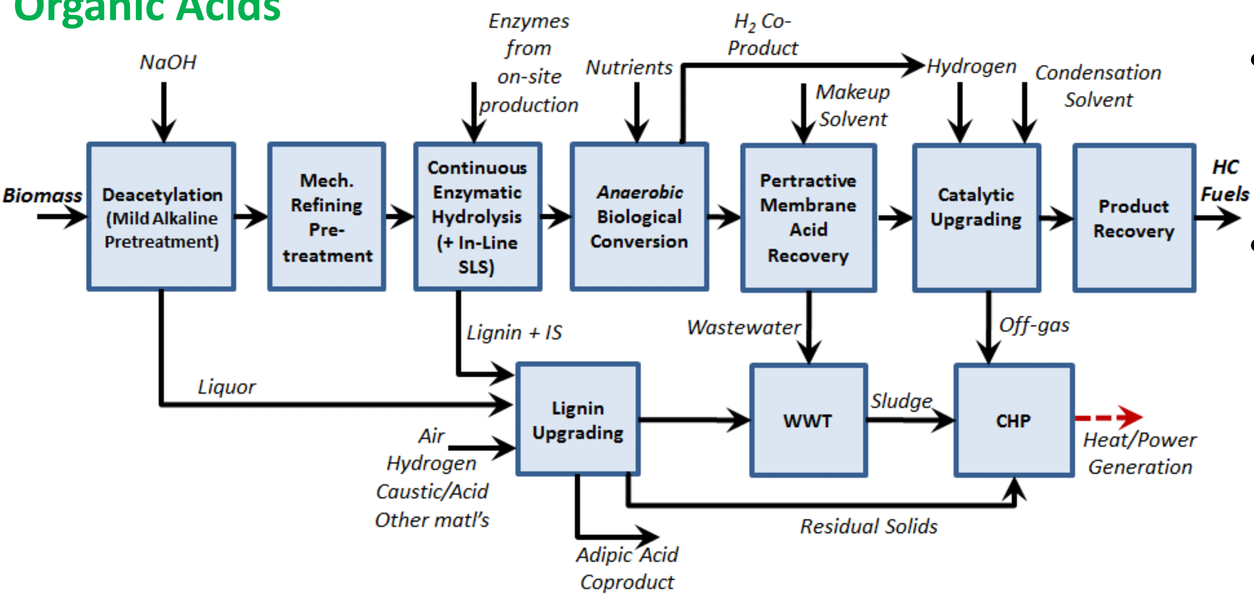
https://www.nrel.gov/docs/fy19osti/71949.pdf

2018 Design Report: Process Configurations

2,3-BDO

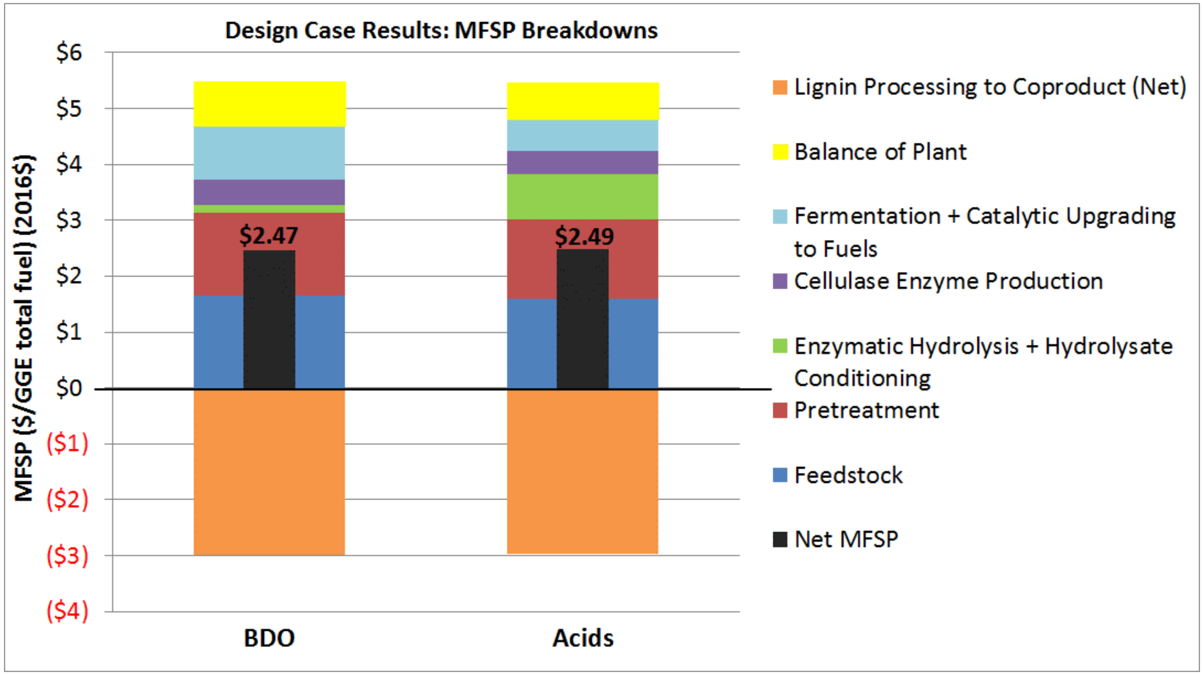


Organic Acids



- Two pathways considered:
  - 2,3-BDO to fuels
  - C4 acids to fuels
- Focused on anaerobic pathways per prior TEA
- Both pathways include lignin deconstruction/upgrading to coproducts (adipic acid as example)
- BDO: Batch EH + whole-slurry fermentation, aqueous upgrading
- Acids: Continuous EH (includes solids removal), clarified sugar fermentation, pertractive acid recovery + upgrading

Design Report: Key Results and Comparisons

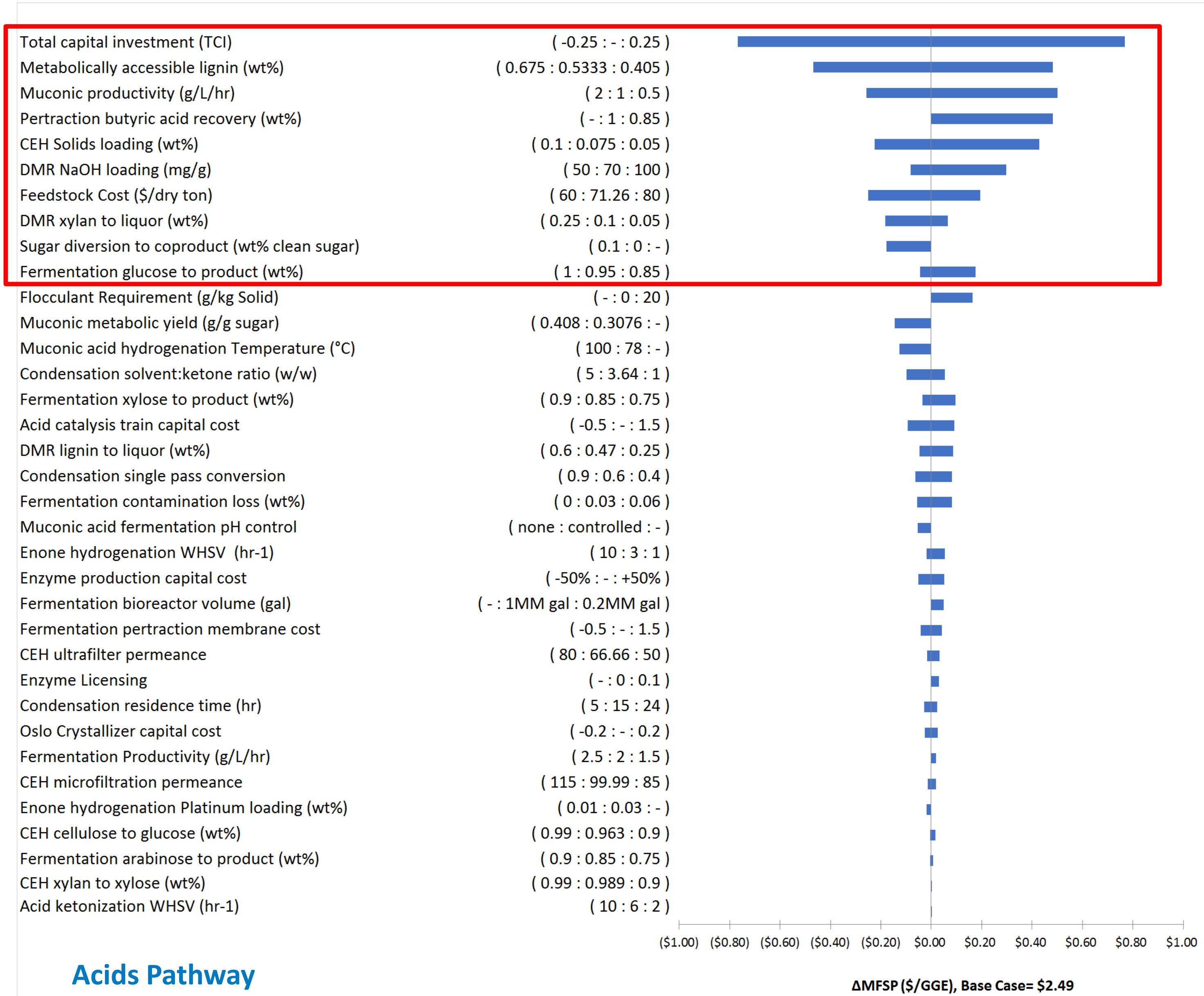


Parameter	BDO Pathway	Acids Pathway
MFSP ($/GGE)	$2.47	$2.49
Fuel Yield (GGE/ton)	43.2	44.8
% Diesel	52%	100%
% Naphtha	48%	0%
Adipic Acid Coproduct Yield (lb/ton)	266	259

- Both pathways exhibit comparable net MFSP results
- Tradeoffs between hydrolysis + hydrolysate processing (more complex/costly for acids) vs fuel upgrading (more costly for BDO w/ 90% water)
- BDO pathway = slightly simpler process, lower overall capex, slightly more C available for coproduct

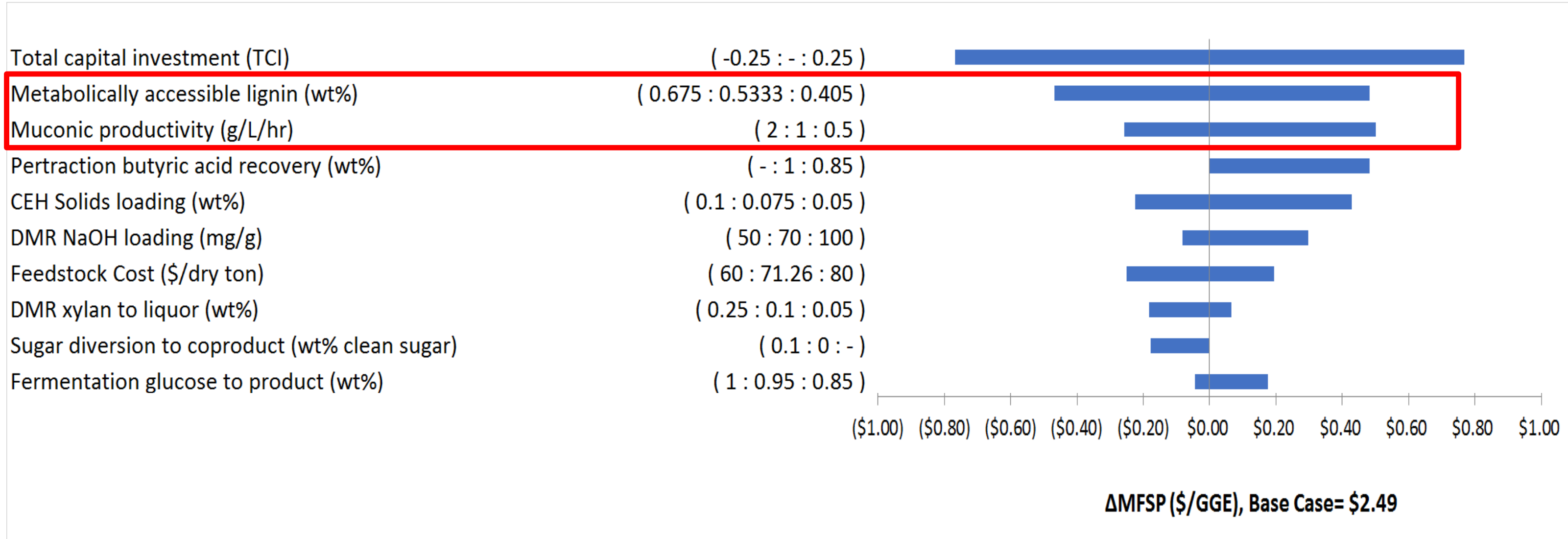
- BDO: Range of products (~C8-C16 alkanes via butene oligomerization)
- Acids: Single target molecule (C14 isomer for jet/diesel via C7 ketone condensation)

Sensitivity Analysis Highlights Key Cost Drivers



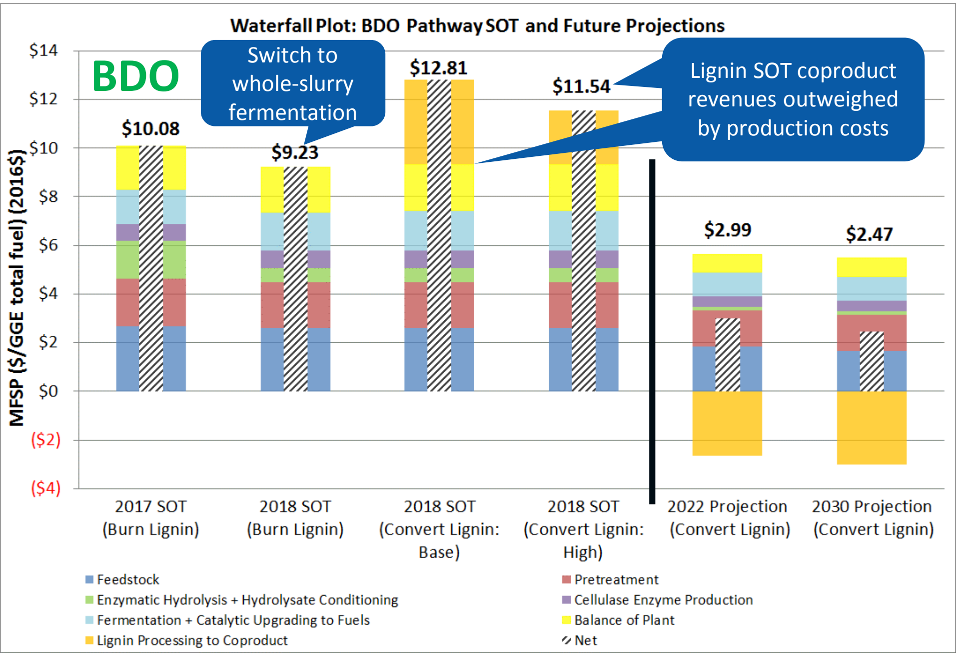
Acids Pathway

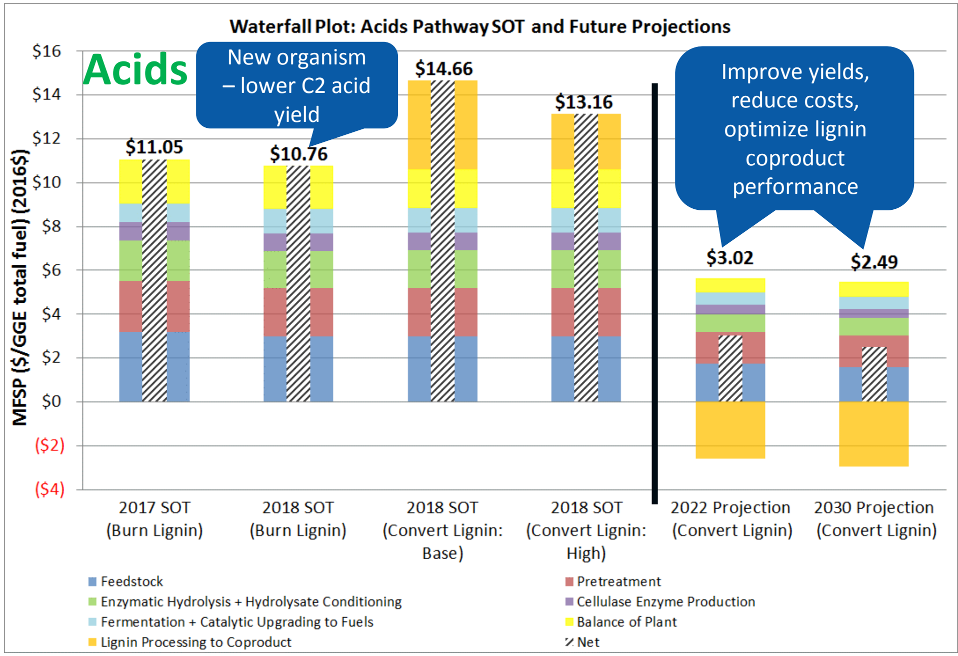
Sensitivity Analysis Highlights Key Cost Drivers



- High CAPEX = high sensitivity to +/- 25% CAPEX accuracy
- Lignin coproduct train exhibits strongest process cost drivers (high value coproduct, but also high production costs) – **lignin conversion yields and aerobic fermentation productivity will be key to enabling MFSP goals**
- Also fuel yields (fermentation recoveries, sugar yields) and process solids loading are important drivers

Technical Accomplishments/Progress/Results: *Benchmarking Progress Through SOTs*





- 2018 SOT benchmarks considered three lignin scenarios:
  - **Burn lignin** (no lignin coproduct inclusion)
  - **Convert lignin (base)** – experimental lignin conversion data on **biomass hydrolysate (0.06 g/L-hr)**
  - **Convert lignin (high)** – experimental lignin conversion data on **model lignin monomers (0.5 g/L-hr)**
- BDO 2018 SOT “burn lignin” = $0.85/GGE improvement vs 2017 SOT – enabled by switch to whole-slurry fermentation (lower costs, no sugar losses)
- 2018 is first year incorporating lignin conversion – low coproduct revenues outweighed by high coproduct process costs = **MFSP penalty vs burning lignin**

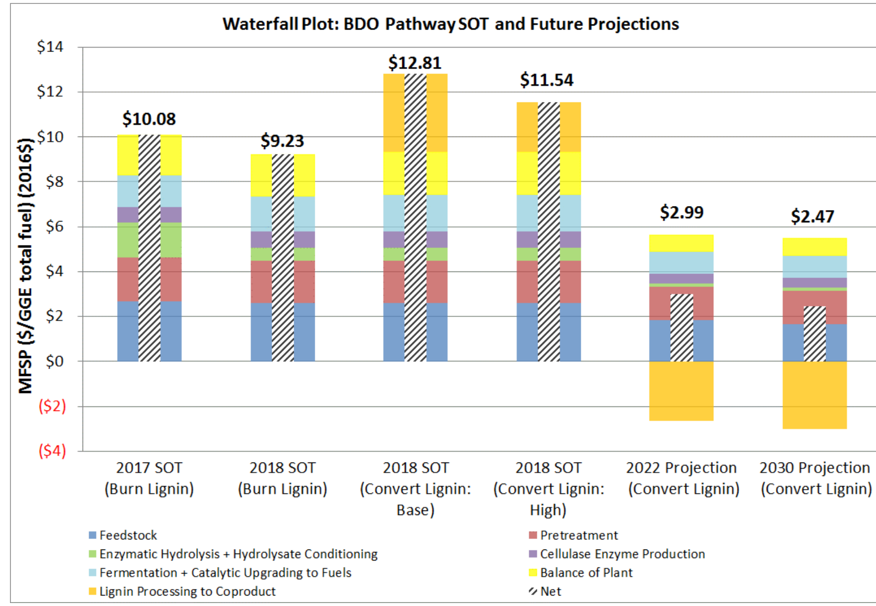
  → ***Significant room to further improve overall lignin conversion + productivity moving forward***

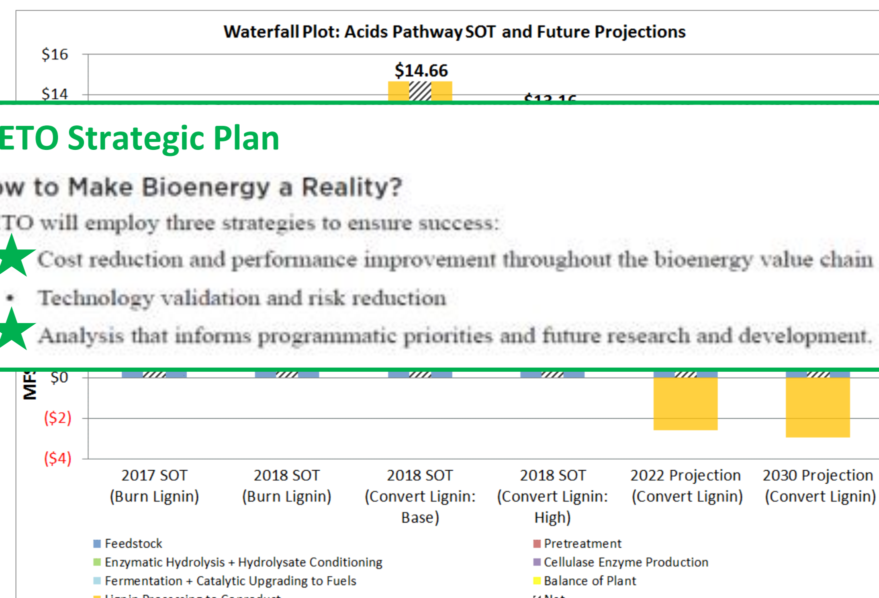
Relevance

TEA is highly relevant to industry + BETO goals:

- Analysis can serve a wide variety of stakeholders
  - *Industry (facilitate interaction with industry, inform investment decisions)*
  - *Research community, decision makers*
  - *Highlight gaps to scale-up/commercialization*
- Identifies key directions (pathways, coproducts)

- **Guides R&D, DOE decisions, sets out year targets**
  - *Technical targets, e.g.:*
    - *Deconstruction: enzyme loadings, sugar yields (LTAD)*
    - *Fermentation: process yields, productivities (BSI/BUS)*
    - *Upgrading: catalyst type, WHSV, lifetime (CUBI)*
    - *Lignin: conversion/upgrading yields (Lignin Upgr.)*
  - *Cost targets (BETO goal: <$2.5/GGE MFSP by 2030)*
- **Public dissemination** of models: e.g. updated 2018 sugar model: https://www.nrel.gov/extranet/biorefinery/aspen-models/





BETO Strategic Plan

How to Make Bioenergy a Reality?

BETO will employ three strategies to ensure success:

- Cost reduction and performance improvement throughout the bioenergy value chain
- Technology validation and risk reduction
- Analysis that informs programmatic priorities and future research and development.

Future Work

- 2018 SOT benchmarking and MYP support *(Q1 FY19, complete):*
  - Complete 2018 SOT benchmarking TEA models and deliver milestone report documenting key input data
  - **Provide information to support MYP** report based on TEA outputs/cost breakdown details
- Modeling for lignin RCF opportunities *(Q2 FY19, joint with Lignin First project):*
  - Conduct preliminary TEA modeling for at least one lignin RCF (reductive catalytic fractionation) concept, as an alternative processing option to the 2018 design case
  - **Identify key barriers and process targets** that would require maintaining $2.5/GGE goals
- Biogas upgrading TEA *(Q3 FY19, collaborative with Biogas Catalysis project):*
  - Evaluate TEA for at least two process configuration options focused on upgrading of waste gas/biogas carbon to fuels or products
  - Consider process implications for this approach as an **alternative risk mitigation strategy** in the event lignin coproduct conversion yields cannot be achieved (requiring AD to be re-introduced)
- Alternative lignin coproducts TEA *(Q3 FY19, collaborative with ORNL 2.3.2.104):*
  - Complete preliminary TEA for alternative lignin coproducts via itaconic acid
  - **Highlight data gaps and key metrics** needed to support MFSP goals
- 2019 SOT and TEA re-benchmarking *(Q4 FY19, inputs from numerous projects):*
  - Conduct 2019 SOT assessment to benchmark latest developments
  - Assist the Platform in re-benchmarking where R&D progress stands relative to prior projections, **highlight largest barriers/risks that must be overcome in gearing up for 2022 $3/GGE demos**

Summary

1) Overview: This project supports BETO by translating R&D into economics using TEA modeling, tracking progress towards future targets
2) Approach: Aspen Plus process modeling coupled with economic analysis. Supports industry via design reports, communication with stakeholders, external collaborations, incorporation of developments from numerous consortia efforts
3) Technical accomplishments: Biochemical Analysis task has seen a tremendous amount of activity and achievements since FY17 peer review
   - Novel dynamic process/TEA modeling approaches for complex fermentations
   - Publication of updated Biochemical Design Report, inputs to support MYP
   - Public release of updated NREL Sugar Model over multiple deconstruction options
   - TEA to guide R&D decisions and benchmark progress for experimental projects
4) Relevance: TEA work is highly relevant to supporting program directions for BETO, near- and long-term R&D priorities for NREL/partners based on cost drivers
5) Future work:
   - Further efforts planned moving forward around evaluating alternative process strategy options that may be pursued to mitigate risks in achieving future 2022-2030 cost goals
   - SOT re-benchmarking to compare progress vs projections, highlight gaps to support 2022 interim demonstrations
   - Continued focus on importance of lignin valorization

Acronyms

- ACM = Aspen Custom Modeler (equation-based models for dynamic bioreactor operation)
- BDO = 2,3-butanediol
- Design case = future technical target projections to achieve TEA cost goals
- GGE = gallon gasoline equivalent
- MFSP = minimum fuel selling price
- MYP = BETO's Multi-Year Plan (formerly MYPP = Multi-Year Program Plan)
- OTR = oxygen transfer rate
- SOT = state-of-technology (annual benchmarking to update TEA based on latest R&D data)
- TEA = techno-economic analysis

Thank You

www.nrel.gov
https://www.nrel.gov/bioenergy/biochemical-processes.html

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Additional Slides

Response to Reviewers' Comments (2017 Review)

- Two important aspects of the project will be the interaction with the individual NREL projects, to support ongoing decision-making (tornado plots to identify higher value targets for cost-reduction), and how the project can provide value to a wider audience of stakeholders. Beyond publishing models it may be worthwhile for the team to consider ways to help companies or other national labs improve their own modeling capabilities, through workshops and provision of tools. Another aspect to consider could be increasing the bandwidth of the team to allow it to provide a fee-for-service offering on similar modeling methods to other BETO funding recipients or outside companies.
- We thank the reviewers for their positive feedback in recognizing the impact of this project for BETO and the utility in guiding R&D priorities for NREL and the community. We do offer a number of different collaboration/"fee-for-service" mechanisms for partners seeking to leverage our TEA capabilities, and have worked with numerous industry and academic groups over recent years to provide TEA/LCA/process modeling support. We also participate in various partnership-outreach functions, and have hosted visitors from industry, academia, and other national labs seeking to work with our TEA modeling group to better understand TEA practice. Additionally, we have made a number of our models publicly available and are working to publish others once they have been properly refined, vetted, and automated for usability.

- It would be helpful to understand exactly how the co-bioproduct target molecules were chosen. It seems that products with higher value and/or larger market could be identified.
- The primary intent of our TEA work in that respect has been to quantitatively demonstrate the benefits that may be gained by introducing coproducts as a means to reduce fuel costs and ultimately enable economic viability in a conceptual biorefinery. To date we have approached this by reflecting coproduct molecules that have been the subject of internal NREL research focus (previously succinic acid from sugars, and more recently adipic acid from lignin) as representative examples to demonstrate proof-of-concept for commercially-relevant high-value bioproducts, which do generally have high market volumes or potential to produce derivative products with high market volumes. This forms a basis upon which industry may build in the future for similar multi-fuel/product biorefinery concepts, recognizing that biorefineries on a national scale would target many different coproduct opportunities based on market drivers at the time.

Publications and Presentations (Since 2017 Review)

- R. Davis, N. Grundl, L. Tao, M.J. Biddy, E.C.D. Tan, G.T. Beckham, D. Humbird, D.N. Thompson, M.S. Roni. Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels and Coproducts: 2018 Biochemical Design Case Update. NREL Technical Report NREL/TP-5100-71949, November 2018. https://www.nrel.gov/docs/fy19osti/71949.pdf
- H. Cai, J. Han, M. Wang, R. Davis, M. Biddy, E. Tan, "Life-cycle analysis of integrated biorefineries with co-production of biofuels and bio-based chemicals: co-product handling methods and implications." *Biofuels, Bioproducts and Biorefining* 12(5): p. 815-833, 2018.
- N.R. Baral, R. Davis, T.H. Bradley, "Supply and value chain analysis of mixed biomass feedstock supply system for lignocellulosic sugar production." *Biofuels, Bioproducts and Biorefining;* DOI: 10.1002/bbb.1975, 2019.
- B. Yang, L. Tao, C.E. Wyman, "Strengths, challenges, and opportunities for hydrothermal pretreatment in lignocellulosic biorefineries." *Biofuels, Bioproducts and Biorefining* 12(1): p. 125-138, 2018.
- J.S. Kruger, N.S. Cleveland, R.Y. Yeap, T. Dong, K.J. Ramirez, N.J. Nagle, A.C. Lowell, G.T. Beckham, J.D. McMillan, M.J. Biddy, "Recovery of fuel-precursor lipids from oleaginous yeast." *ACS Sustainable Chemistry & Engineering* 6(3): p. 2921-2931, 2018.
- D. Humbird, R. Davis, J.D. McMillan, "Aeration costs in stirred-tank and bubble column bioreactors." *Biochemical Engineering Journal* 127: p. 161-166, 2017.

Backup Slides

BDO Pathway Technical Target Table: SOT + Out-Years

	Units	2017 SOT	2018 SOT	2018 SOT	2018 SOT	2022 Projection	2030 Projection
Lignin Handling	-	**Burn Lignin**	**Burn Lignin**	**Convert Lignin (Base)** [1]	**Convert Lignin (High)** [1]	**Convert Lignin**	**Convert Lignin**
Projected Minimum Fuel Selling Price	**$/GGE**	**$10.08**	**$9.23**	**$12.81**	**$11.54**	**$2.99**	**$2.47**
Feedstock Contribution	$/GGE	$2.67	$2.59	$2.59	$2.59	$1.83	$1.65
Conversion Contribution	**$/GGE**	**$7.41**	**$6.64**	**$10.22**	**$8.95**	**$1.16**	**$0.82**
Total Gasoline Equivalent Yield	GGE/dry U.S. ton	31.4	32.3	32.3	32.3	43.2	43.2
Adipic Acid Coproduct Yield	lb/dry ton biomass	0	0	40	40	235	266
Feedstock							
Feedstock Cost [2]	$/dry U.S. ton	$83.90	$83.67	$83.67	$83.67	$79.07	$71.26
Pretreatment							
Temperature	°C	92	92	92	92	92	92
Residence Time	min	60 (batch)	60 (batch)	60 (batch)	60 (batch)	90 (continuous)	90 (continuous)
Total Caustic (NaOH) Loading	mg/g dry biomass	70	70	70	70	70	70
Net solubilized lignin to liquor	%	47%	47%	47%	47%	47%	47%
Net solubilized glucan to liquor	%	2%	2%	2%	2%	2%	2%
Net solubilized xylan to liquor	%	17%	17%	17%	17%	10%	10%
Net solubilized arabinan to liquor	%	46%	46%	46%	46%	30%	30%
Enzymatic Hydrolysis							
Hydrolysis Configuration	Batch vs CEH	Batch	Batch	Batch	Batch	Batch	Batch
Total Solids Loading to Hydrolysis	wt%	20%	20%	20%	20%	25%	25%
Enzymatic Hydrolysis Batch Time	days	5	5	5	5	5	5
Hydrolysis Glucan to Glucose	%	78%	78%	78%	78%	90%	90%
Hydrolysis Xylan to Xylose	%	85%	85%	85%	85%	90%	90%
Sugar Loss (into solid stream after EH separation)	%	5%	NA (whole slurry)	NA (whole slurry)	NA (whole slurry)	NA (whole slurry)	NA (whole slurry)
Cellulase Enzyme Production							
Enzyme Loading	mg/g cellulose	12	12	12	12	10	10
Fermentation, Catalytic Conversion, and Upgrading to Fuels							
Bioconversion Volumetric Productivity	g/L/hour	1.7	1.1	1.1	1.1	2.6	2.6
Glucose to Product [total glucose utilization] [3]	%	86% [100%]	95% [100%]	95% [100%]	95% [100%]	95% [98%]	95% [98%]
Xylose to Product [total xylose utilization] [3]	%	89% [97%]	90% [92%]	90% [92%]	90% [92%]	90% [92%]	90% [92%]
Arabinose to Product [total arabinose utilization] [3]	%	0% [0%]	0% [0%]	0% [0%]	0% [0%]	85% [89%]	85% [89%]
Bioconversion Metabolic Yield (Process Yield)	g/g sugars	0.44 (0.42)	0.48 (0.46)	0.48 (0.46)	0.48 (0.46)	0.47 (0.45)	0.47 (0.45)
Fermentation intermediate product recovery	wt%	99.7%	96.8%	96.8%	96.8%	96.4%	96.4%
Aqueous BDO Upgrading: WHSV	hr^{-1}	1.0	1.0	1.0	1.0	2.0	2.0
Oligomerization: WHSV	hr^{-1}	1.0	1.0	1.0	1.0	1.0	1.0
Hydrotreating: WHSV	hr^{-1}	5.0	5.0	5.0	5.0	5.0	5.0
Lignin Processing to Coproduct							
Solid Deconstruction to Soluble Lignin	wt% BCD lignin feed	-	-	85%[5]	85%[5]	43%	53%
Convertible Components in Soluble Lignin	wt% of total soluble lignin (APL +BCD)	-	-	16%	16%	98%	98%
Muconic Acid Process Yield from Lignin	g/g soluble lignin	-	-	0.15	0.15	1.75	1.59
Muconic Acid Metabolic Yield from Lignin	g/g lignin consumed	-	-	0.93	0.93	0.93	0.93
Overall Carbon Upgrading Efficiency to Coproduct [4]	mol%	-	-	3.8%	3.8%	24.5%	27.8%
Muconic Acid Productivity	g/L/hr	-	-	0.06	0.53	1.0	1.0

Acids Pathway Technical Target Table: SOT + Out-Years

	Units	2017 SOT	2018 SOT	2018 SOT	2018 SOT	2022 Projection	2030 Projection
Lignin Handling	-	**Burn Lignin**	**Burn Lignin**	**Convert Lignin (Base)** [1]	**Convert Lignin (High)** [1]	**Convert Lignin**	**Convert Lignin**
Projected Minimum Fuel Selling Price	**$/GGE**	**$11.05**	**$10.76**	**$14.66**	**$13.16**	**$3.02**	**$2.49**
Feedstock Contribution	$/GGE	$3.19	$2.99	$2.99	$2.99	$1.76	$1.59
Conversion Contribution	**$/GGE**	**$7.86**	**$7.77**	**$11.67**	**$10.17**	**$1.26**	**$0.90**
Total Gasoline Equivalent Yield	GGE/dry U.S. ton	26.3	28.0	28.0	28.0	44.8	44.8
Adipic Acid Coproduct Yield	lb/dry ton biomass	0	0	41	41	229	259
Feedstock							
Feedstock Cost [2]	$/dry U.S. ton	$83.90	$83.67	$83.67	$83.67	$79.07	$71.26
Pretreatment							
Temperature	°C	92	92	92	92	92	92
Residence Time	min	60 (batch)	60 (batch)	60 (batch)	60 (batch)	90 (continuous)	90 (continuous)
Total Caustic (NaOH) Loading	mg/g dry biomass	70	70	70	70	70	70
Net solubilized lignin to liquor	%	47%	47%	47%	47%	47%	47%
Net solubilized glucan to liquor	%	2%	2%	2%	2%	2%	2%
Net solubilized xylan to liquor	%	17%	17%	17%	17%	10%	10%
Net solubilized arabinan to liquor	%	46%	46%	46%	46%	30%	30%
Enzymatic Hydrolysis							
Hydrolysis Configuration	Batch vs CEH	Batch	Batch	Batch	Batch	CEH	CEH
Total Solids Loading to Hydrolysis	wt%	20%	20%	20%	20%	7.6%	7.6%
Enzymatic Hydrolysis Batch Time	days	5	5	5	5	Continuous	Continuous
Hydrolysis Glucan to Glucose	%	78%	78%	78%	78%	96%	96%
Hydrolysis Xylan to Xylose	%	85%	85%	85%	85%	99%	99%
Sugar Loss (into solid stream after EH separation)	%	5%	5%	5%	5%	1%	1%
Cellulase Enzyme Production							
Enzyme Loading	mg/g cellulose	12	12	12	12	10	10
Fermentation, Catalytic Conversion, and Upgrading to Fuels							
Bioconversion Volumetric Productivity	g/L/hour	1.1	0.3	0.3	0.3	2.0	2.0
Glucose to Product [total glucose utilization] [3]	%	86% [100%]	90% [95%]	90% [95%]	90% [95%]	95% [100%]	95% [100%]
Xylose to Product [total xylose utilization] [3]	%	82% [100%]	77% [90%]	77% [90%]	77% [90%]	85% [100%]	85% [100%]
Arabinose to Product [total arabinose utilization] [3]	%	82% [100%]	32% [38%]	32% [38%]	32% [38%]	85% [87%]	85% [87%]
Bioconversion Metabolic Yield (Process Yield)	g/g sugars	0.44 (0.44)	0.45 (0.41)	0.45 (0.41)	0.45 (0.41)	0.45 (0.43)	0.45 (0.43)
Fermentation intermediate product recovery	wt%	60% (C2), 95% (C4)	60% (C2), 95% (C4)	60% (C2), 95% (C4)	60% (C2), 95% (C4)	100% (C4)	100% (C4)
Ketonization: WHSV	hr^{-1}	6.0	4.0	4.0	4.0	6.0	6.0
Condensation: WHSV	hr^{-1}	0.5	10 hr batch	10 hr batch	10 hr batch	15 hr batch	15 hr batch
Hydrotreating: WHSV	hr^{-1}	3.0	4.7	4.7	4.7	3.0	3.0
Lignin Processing to Coproduct							
Solid Deconstruction to Soluble Lignin	wt% BCD lignin feed	-	-	85%[5]	85%[5]	43%	53%
Convertible Components in Soluble Lignin	wt% of total soluble lignin (APL +BCD)	-	-	16%	16%	98%	98%
Muconic Acid Process Yield from Lignin	g/g soluble lignin	-	-	0.15	0.15	1.75	1.59
Muconic Acid Metabolic Yield from Lignin	g/g lignin consumed	-	-	0.93	0.93	0.93	0.93
Overall Carbon Upgrading Efficiency to Coproduct [4]	mol%	-	-	4.0%	4.0%	26.7%	30.1%
Muconic Acid Productivity	g/L/hr			0.06	0.52	1.0	1.0

Comparison of Key SOT Metrics: BDO vs Acids Pathways

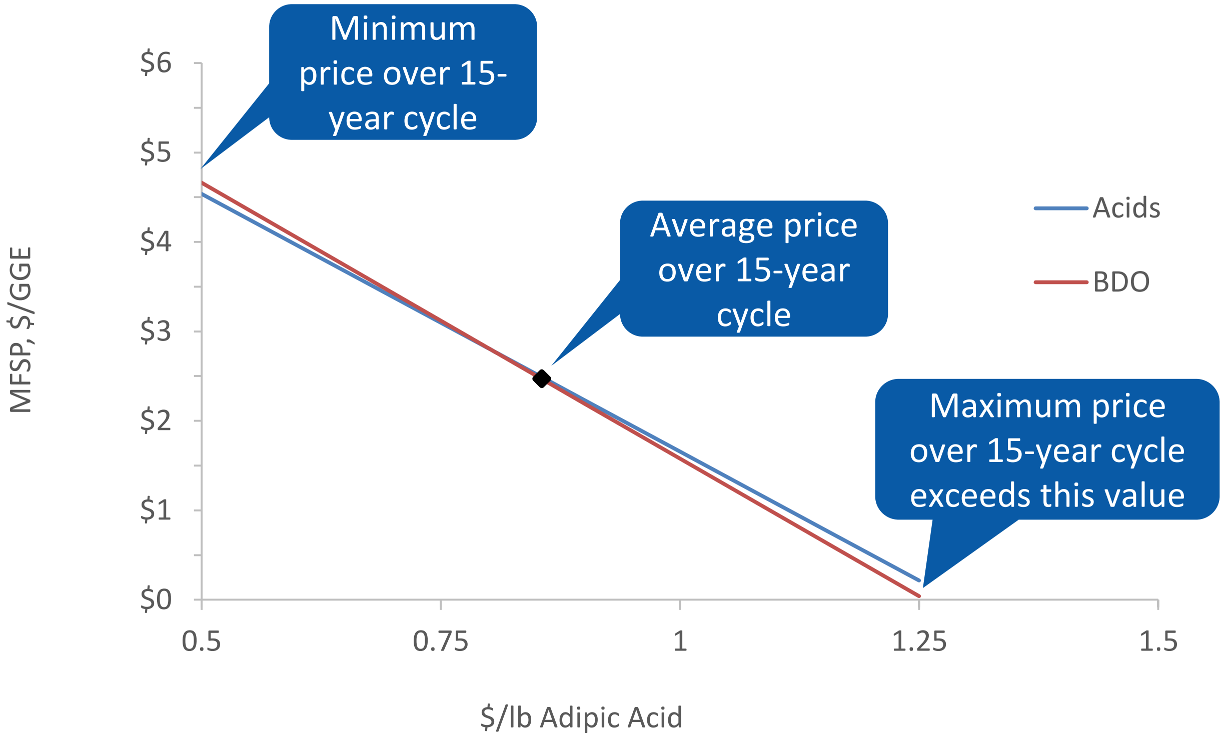
	Units	2017 SOT	2018 SOT	2018 SOT	2018 SOT	2022 Projection	2030 Projection
Lignin Handling	-	**Burn Lignin**	**Burn Lignin**	**Convert Lignin (Base)**	**Convert Lignin (High)**	**Convert Lignin**	**Convert Lignin**
BDO Pathway							
Minimum Fuel Selling Price	**$/GGE**	**$10.08**	**$9.23**	**$12.81**	**$11.54**	**$2.99**	**$2.47**
Feedstock Contribution	$/GGE	$2.67	$2.59	$2.59	$2.59	$1.83	$1.65
Conversion Contribution	**$/GGE**	**$7.41**	**$6.64**	**$10.22**	**$8.95**	**$1.16**	**$0.82**
Total Gasoline Equivalent Yield	GGE/dry U.S. ton	31.4	32.3	32.3	32.3	43.2	43.2
Adipic Acid Coproduct Yield	lb/dry ton biomass	0	0	40	40	235	266
Adipic Acid Fermentation Productivity	g/L-hr	NA	NA	0.06	0.53	1.0	1.0
Acids Pathway							
Minimum Fuel Selling Price	**$/GGE**	**$11.05**	**$10.76**	**$14.66**	**$13.16**	**$3.02**	**$2.49**
Feedstock Contribution	$/GGE	$3.19	$2.99	$2.99	$2.99	$1.76	$1.59
Conversion Contribution	**$/GGE**	**$7.86**	**$7.77**	**$11.67**	**$10.17**	**$1.26**	**$0.90**
Total Gasoline Equivalent Yield	GGE/dry U.S. ton	26.3	28.0	28.0	28.0	44.8	44.8
Adipic Acid Coproduct Yield	lb/dry ton biomass	0	0	41	41	229	259
Adipic Acid Fermentation Productivity	g/L-hr	NA	NA	0.06	0.53	1.0	1.0

Sustainability Indicators (Conversion Models): SOT + Out-Years

	2017 SOT (Burn Lignin)	2018 SOT (Burn Lignin)	2018 SOT Convert Lignin (Base)	2018 SOT Convert Lignin (High)	2022 Projection (Convert Lignin)	2030 Projection (Convert Lignin)
BDO Pathway:						
Fuel Yield by Weight of Biomass (wt% of dry biomass)	9.6%	9.9%	9.9%	9.9%	13.2%	13.2%
Carbon Efficiency to Fuels (% C in feedstock)	18.2%	18.7%	18.7%	18.7%	25.0%	25.0%
Carbon Efficiency to Lignin Coproduct (% C in feedstock)	NA	NA	2.3%	2.3%	13.1%	14.8%
Net Electricity Import (KWh/GGE)	12.3	10.2	14.0	14.0	10.1	10.5
Net Natural Gas Import (BTU/GGE [LHV])	0	0	75,284	76,789	5,614	14,596
Water Consumption (gal water/GGE)	23.4	9.5	11.3	11.5	8.4	8.9
Acids Pathway:						
Fuel Yield by Weight of Biomass (wt% of dry biomass)	8.1%	8.6%	8.6%	8.6%	13.8%	13.8%
Carbon Efficiency to Fuels (% C in feedstock)	15.5%	16.3%	16.3%	16.3%	26.2%	26.2%
Carbon Efficiency to Lignin Coproduct (% C in feedstock)	NA	NA	2.3%	2.3%	12.7%	14.4%
Net Electricity Import (KWh/GGE)	5.8	9.1	21.5	21.6	9.6	10.7
Net Natural Gas Import (BTU/GGE [LHV])	0	15,790	15,790	15,790	9,055	9,055
Water Consumption (gal water/GGE)	30.7	31.0	26.0	26.1	13.7	13.5

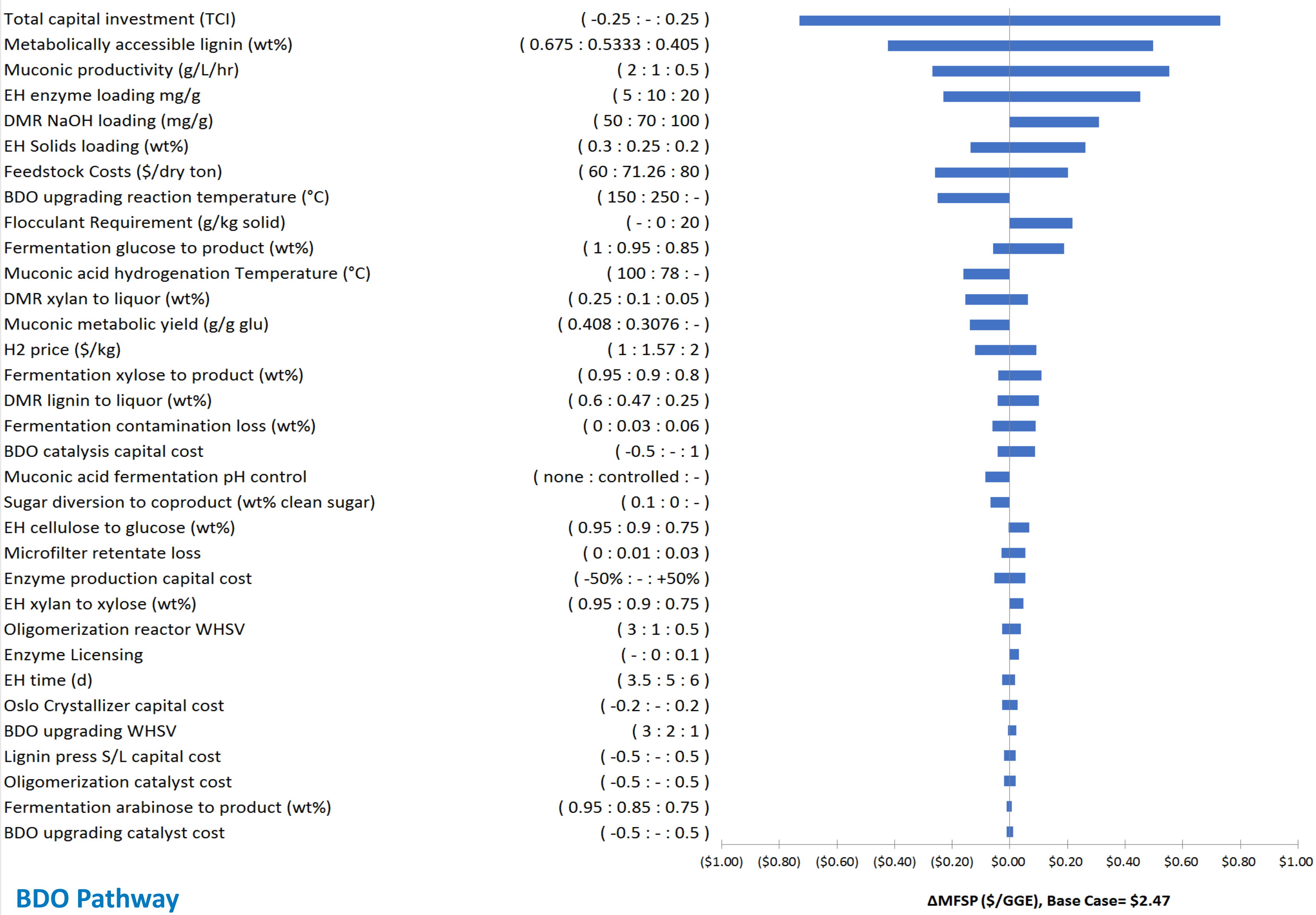
- Project also tracks sustainability indicators based on metrics available directly from Aspen conversion models
- Metrics include mass yield to fuels, carbon yield to fuels and coproducts, energy balances (power and natural gas imports), and water consumption
- Additionally, detailed input/output inventories from process models are furnished to partners at ANL for system LCA modeling

2018 Design Case: MFSP Sensitivity to Adipic Acid Price



- Economics are strongly tied to adipic acid coproduct value (typical for biorefinery models with high-value coproducts)
- To mitigate impacts from price swings, TEA used a 15-year price history for adipic acid at $0.86/lb (recent prices have been lower than this partially tied to petroleum price; but this basis is consistent with future forecasted petroleum price projections over next 30 years)

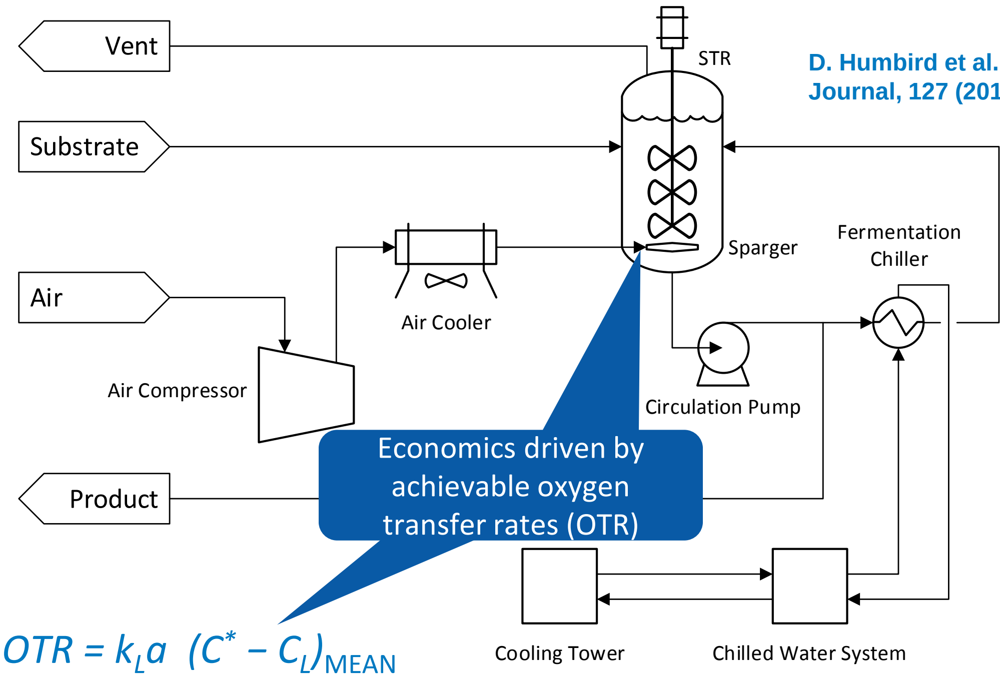
2018 Design Case: BDO Pathway Tornado Chart



BDO Pathway

Technical Accomplishments/Progress/Results: *TEA Highlights Drivers for Aerobic Bioconversion*

D. Humbird et al., Biochemical Engineering Journal, 127 (2017) 161-166



$OTR = k_L a \ (C^* - C_L)_{MEAN}$

STR: $k_L a \ [s^{-1}] = 0.002 \ (P / V \ [W/m^3])^{0.7} \ (u_S \ [m/s])^{0.2}$

BCR: $k_L a \ [s^{-1}] = 0.32 \ (u_S \ [m/s])^{0.7} \ (\mu_{eff} \ [cP])^{-0.84} \ X \ 1.025^{(T\ [°C] - 20)}$

- Aerobic bioconversion costs driven by:
  - Cost to deliver/solubilize oxygen (increases as fermentation becomes more strongly aerobic/higher OUR)
  - Economies of scale: 1,000 m^3 max vessel size in practice today (plausibly up to 2,000 m^3 possible) versus 1 MM gal (~3,800 m^3) for anaerobic = 2–4X more vessels required for same productivity

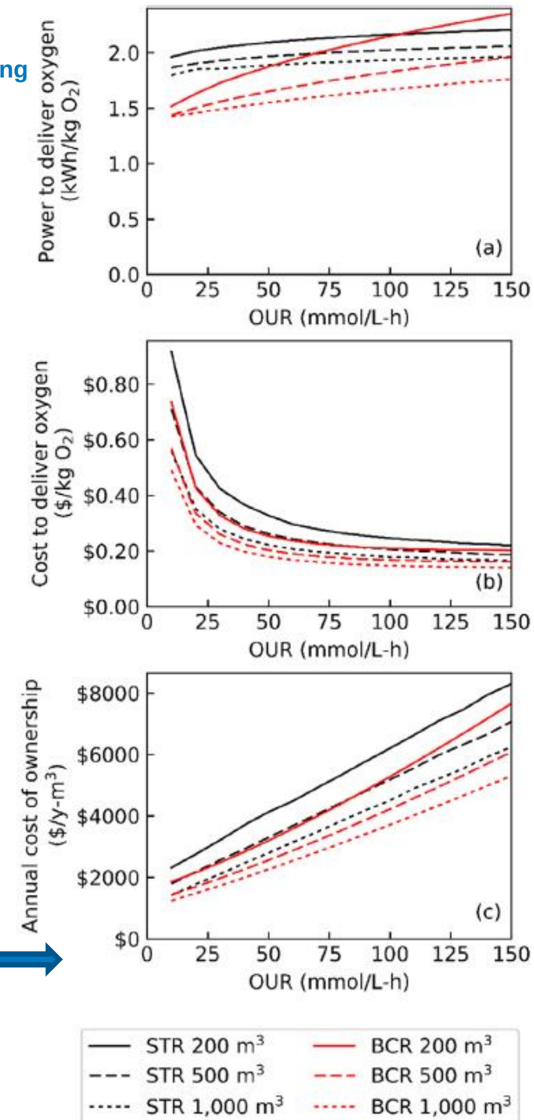
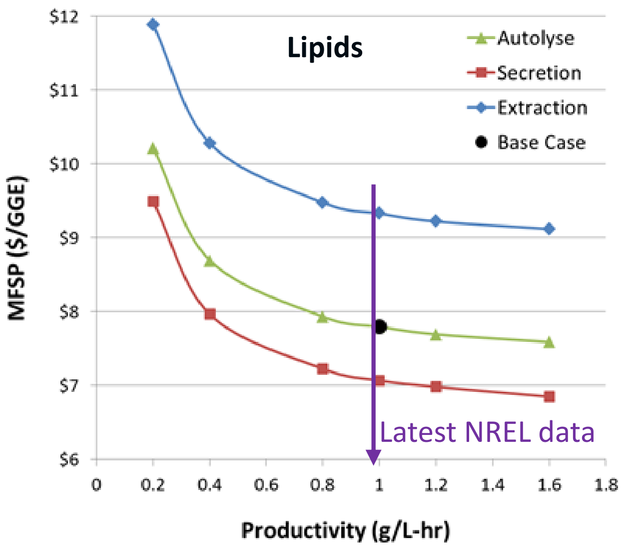
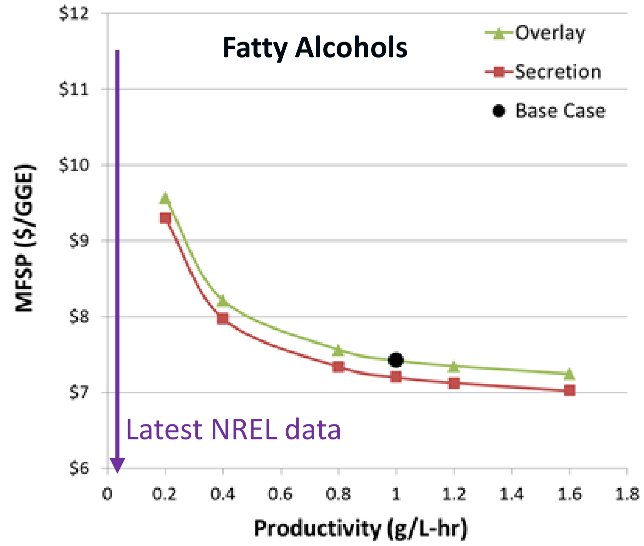


Fig. 3. (a) Specific total power demand, (b) specific aggregate capital and operating cost and (c) annual aggregate capital and operating cost to deliver oxygen in STR and BCR systems at varying vessel volume and OUR.

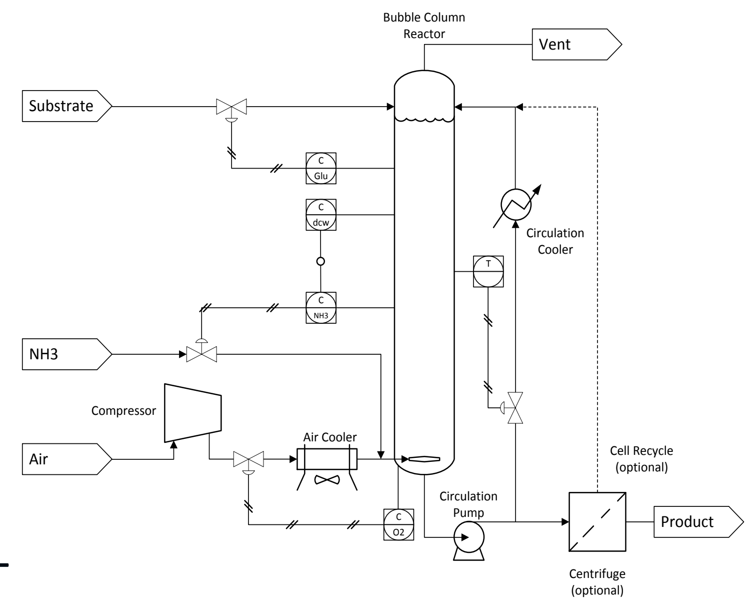
Aerobic Bioconversion: Progress and Barriers





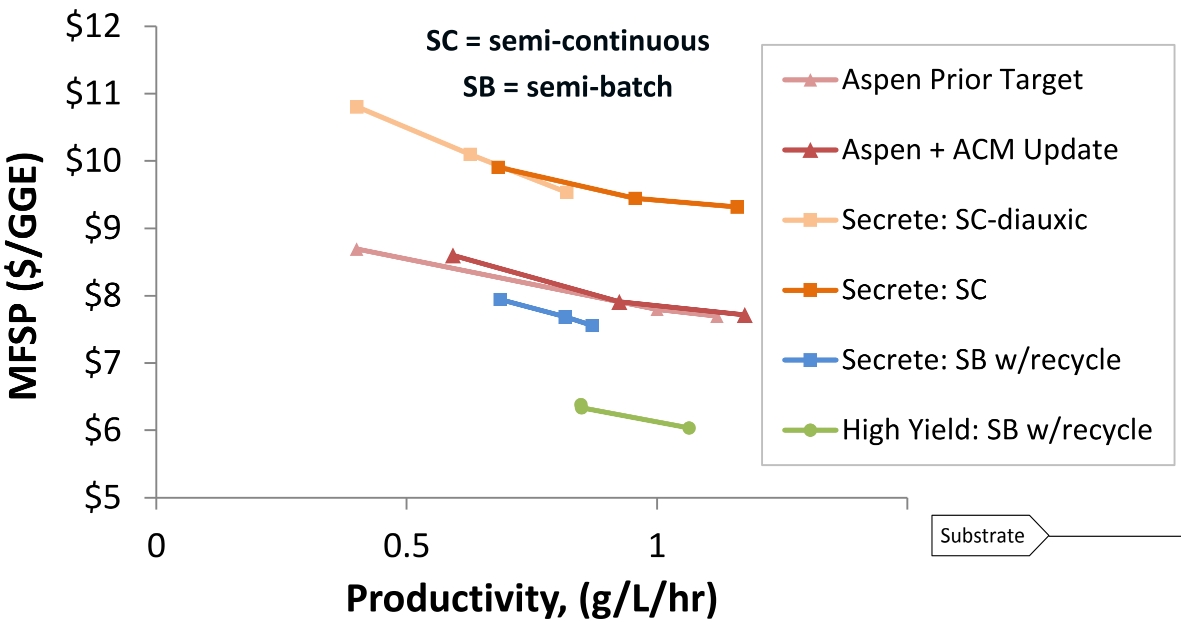
Sensitivity scans based on routing all lignin to boiler (not including lignin coproducts for final MFSP goals)

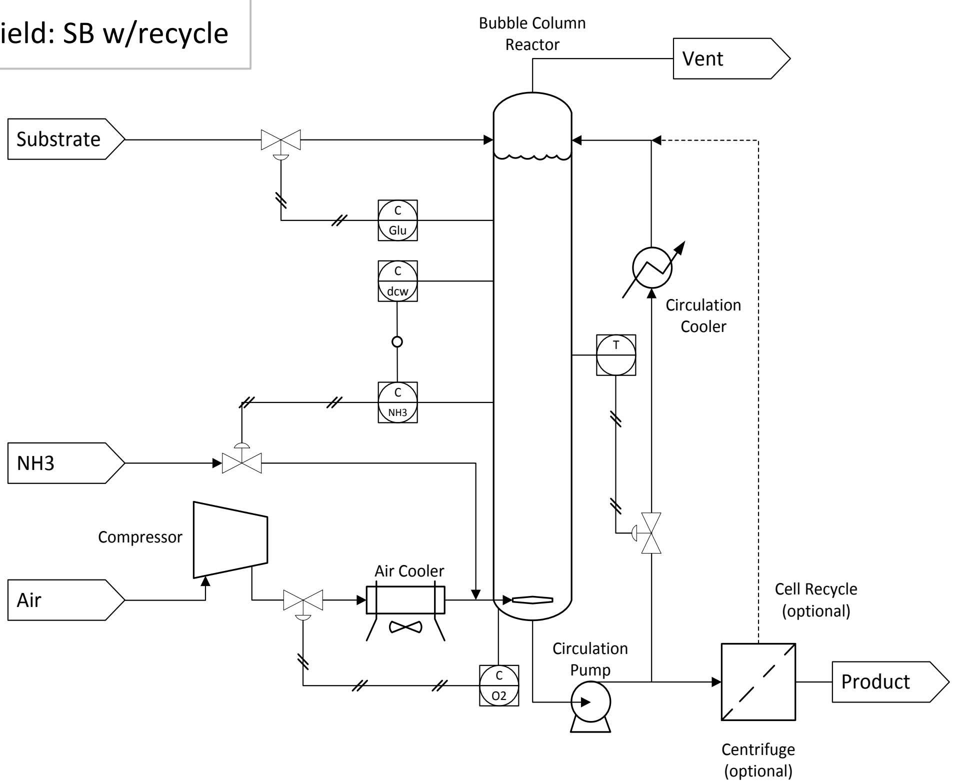
- Fatty Alcohols: Much earlier R&D, more risk to achieving future targets
- Lipids: Significant progress over 5 years, latest data near final targets – BUT, key challenge to achieve cell autolysis for lipid recovery
- Even if autolysis could be achieved, still ~$2/GGE higher than anaerobic options
- TEA findings further validated with new ACM models – better tracking of aerobic fermentor dynamics (OTR, cell vs lipid growth, N inputs over fed-batch cycle)



ACM model for aerobic bubble column (built in consultation with Genomatica)

ACM Modeling: Deeper Dive into Aerobic Bioreactor Dynamics

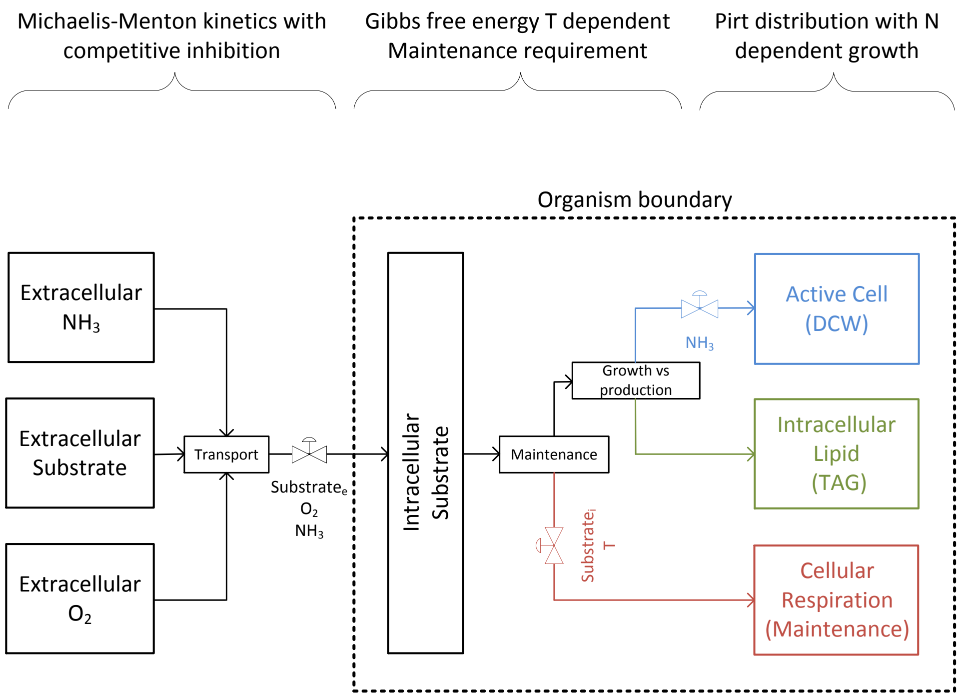




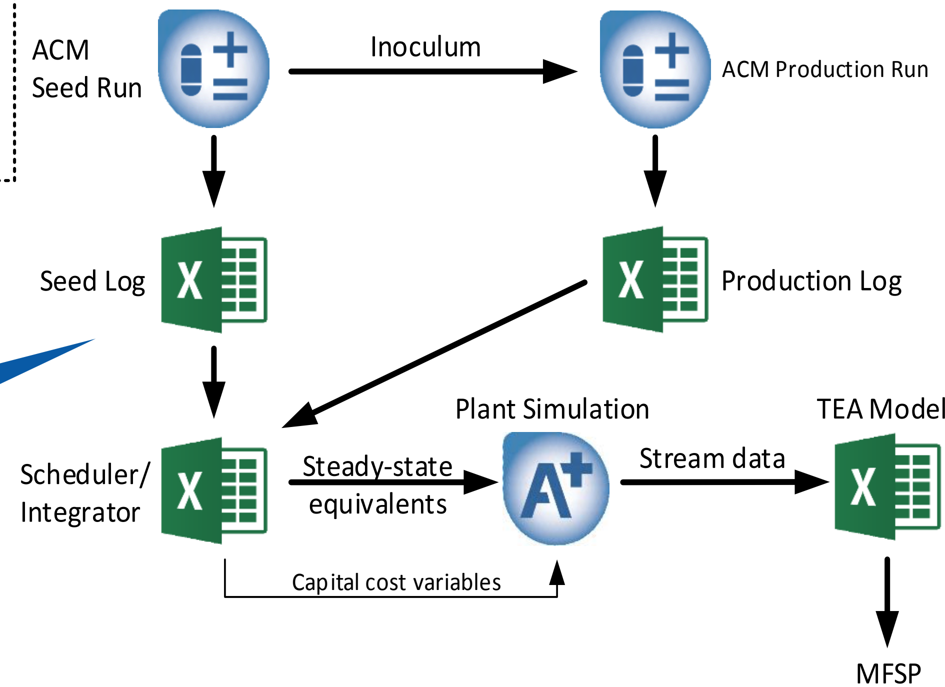
ACM Modeling

- More rigorous model to track dynamics of OTR, cell vs lipid growth, N inputs over fed-batch cycle
- Developed with industry experts
- Validated overall MFSP estimates from Aspen Plus basis over key productivity range – further supports aerobic MFSP conclusions
- Also evaluated alternative bioconversion scenarios; found opportunity to reduce MFSPs closer to anaerobic for longer-range future case (but would require secretion, cell recycle, and higher theoretical yields)

ACM Modeling for Aerobic Fermentation

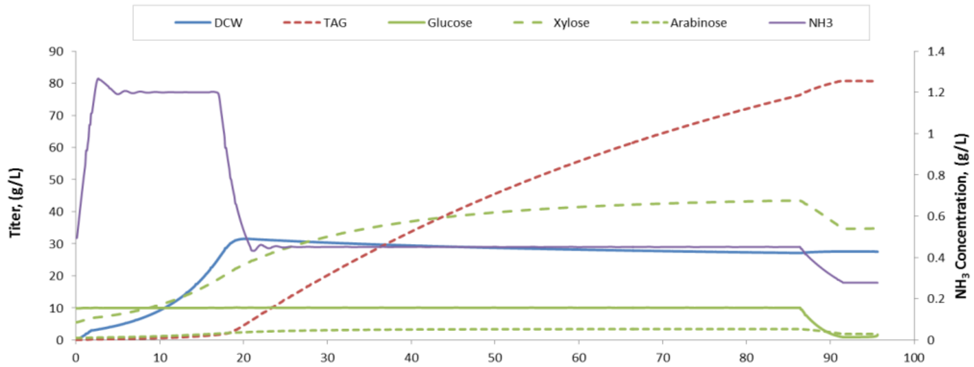


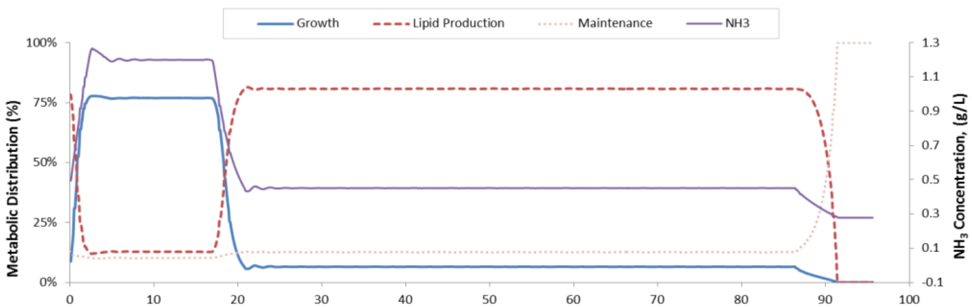
Black box cellular metabolic model included in ACM model

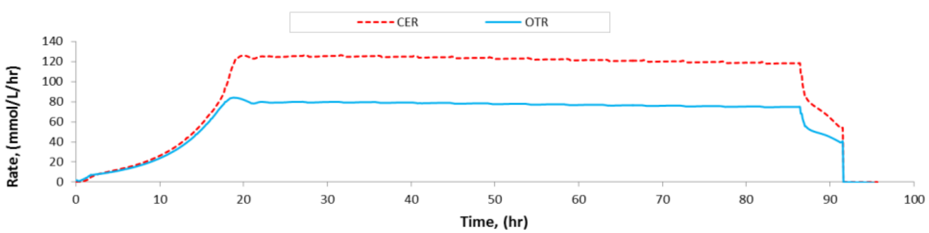


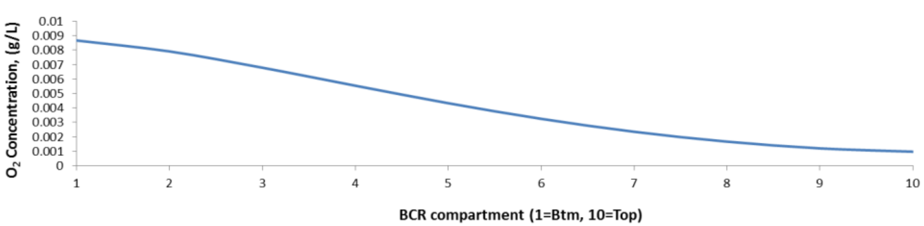
Integration of (dynamic) ACM mechanics into greater (steady state) Aspen Plus model framework

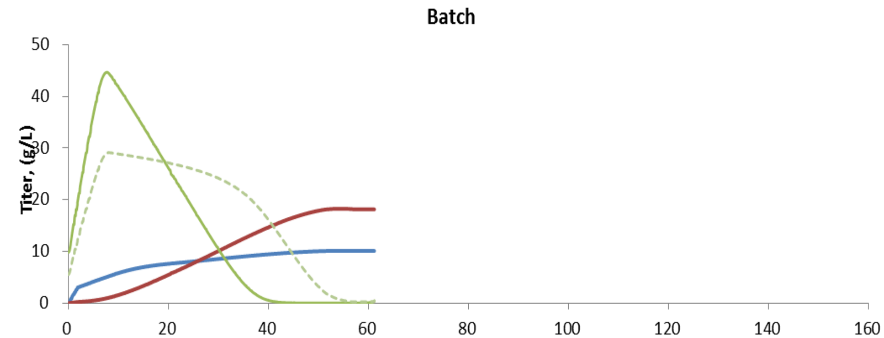
ACM Model: Example Parameters Tracked Over a Run

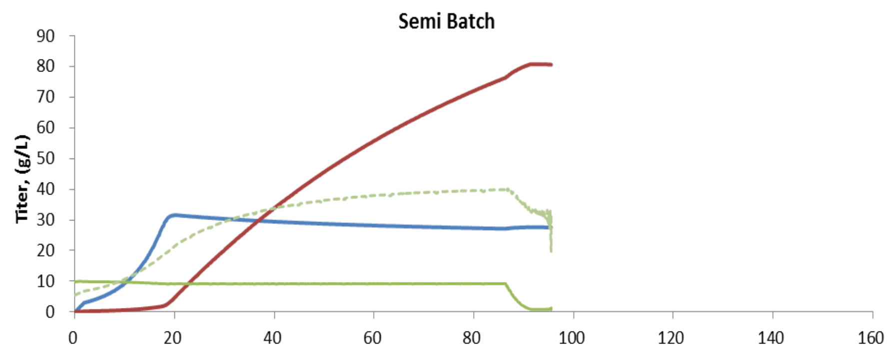


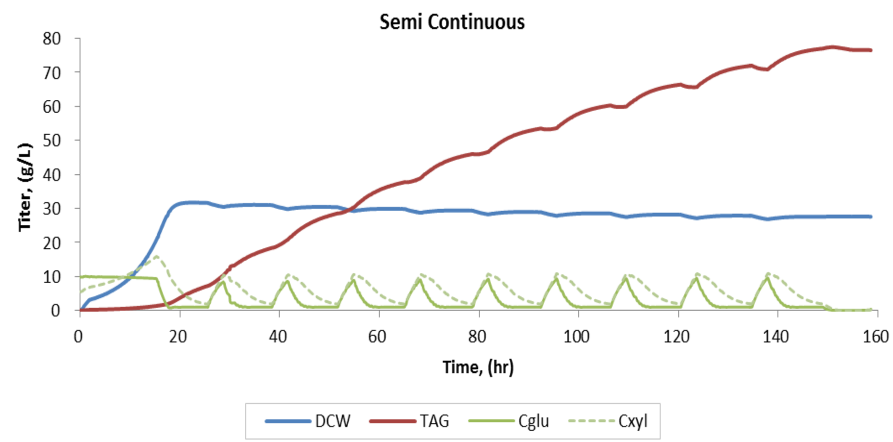








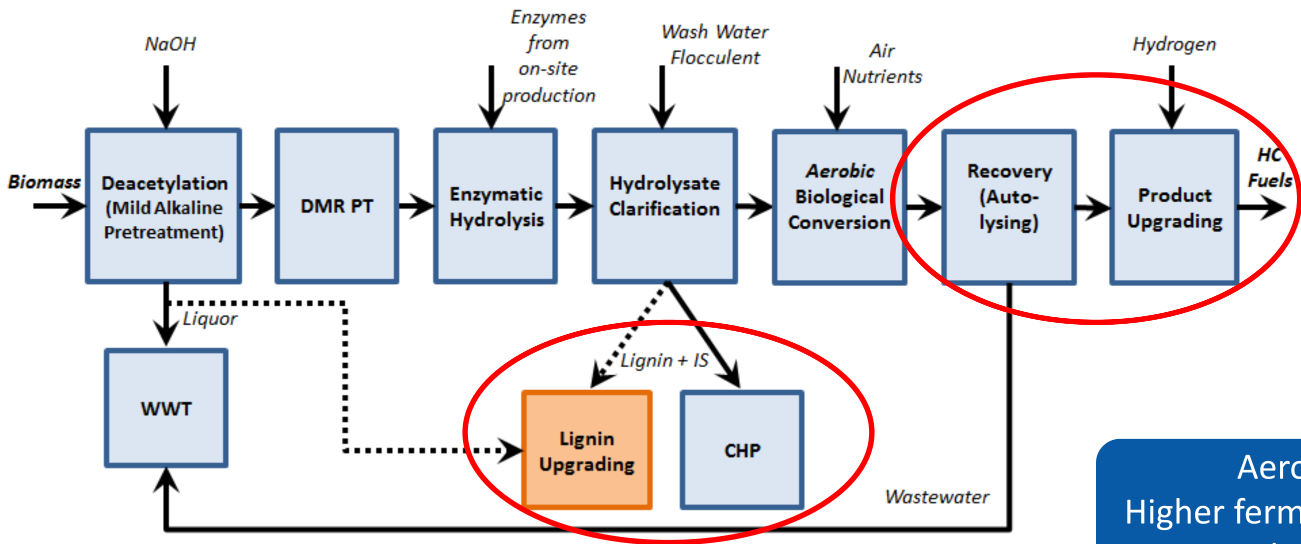




Representative Pathways: Aerobic

Lipids

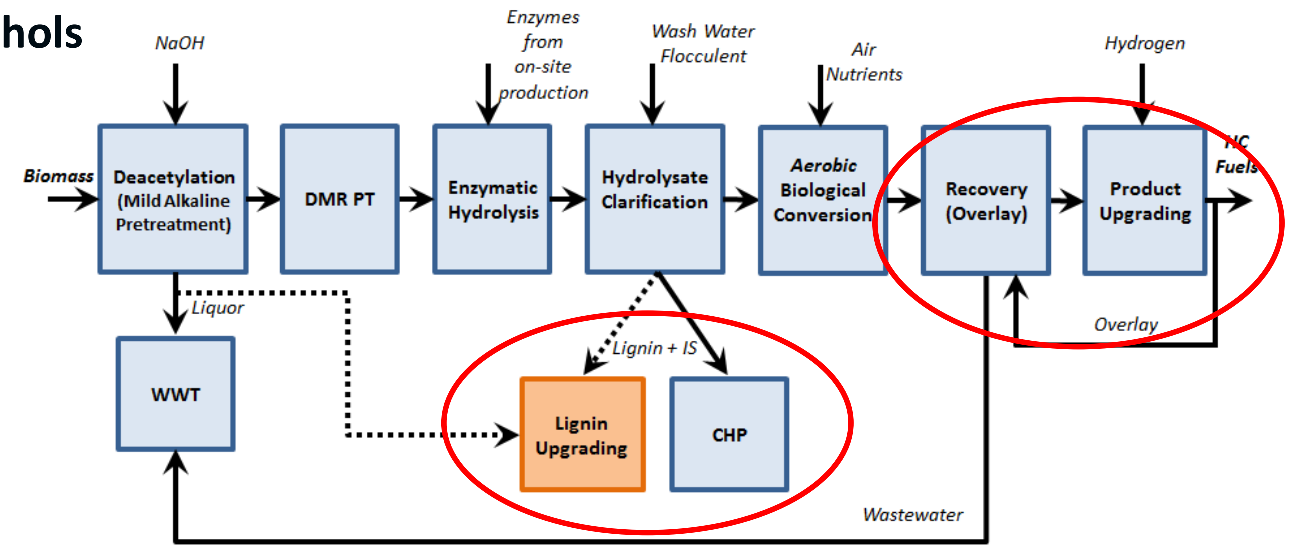
(BSI, PSI, BUS)



Aerobic pathways:
Higher fermentation costs, easier upgrading (long-chain HCs)

Fatty Alcohols

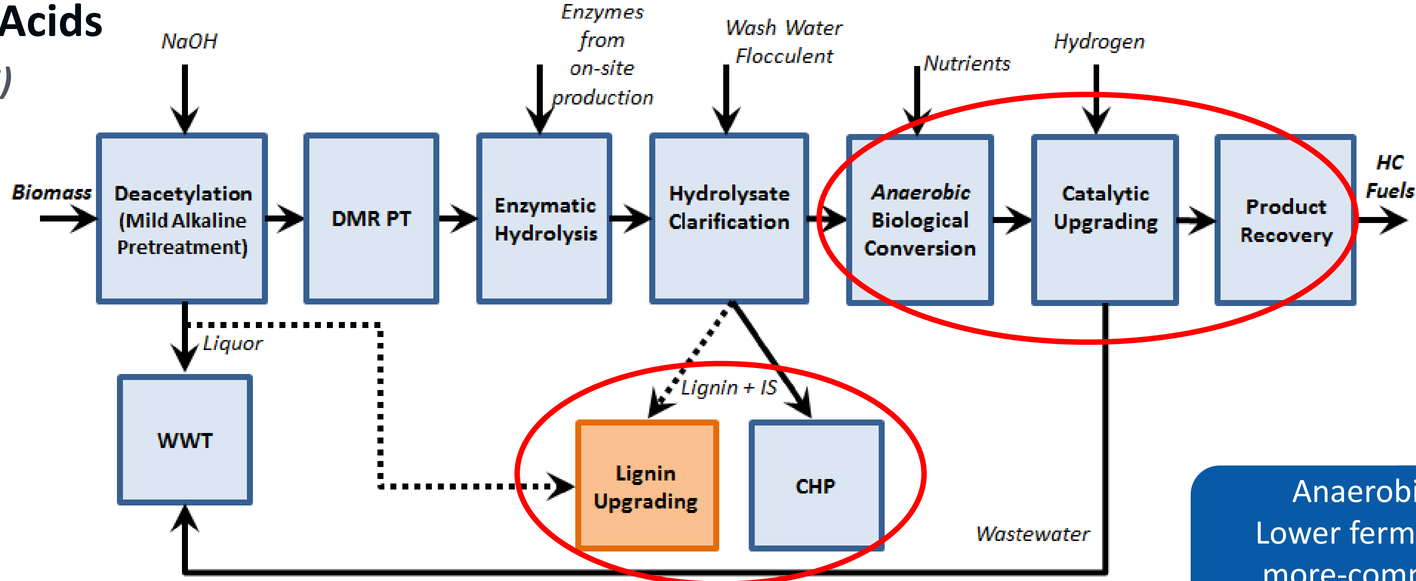
(TMD)



Representative Pathways: Anaerobic

Organic Acids

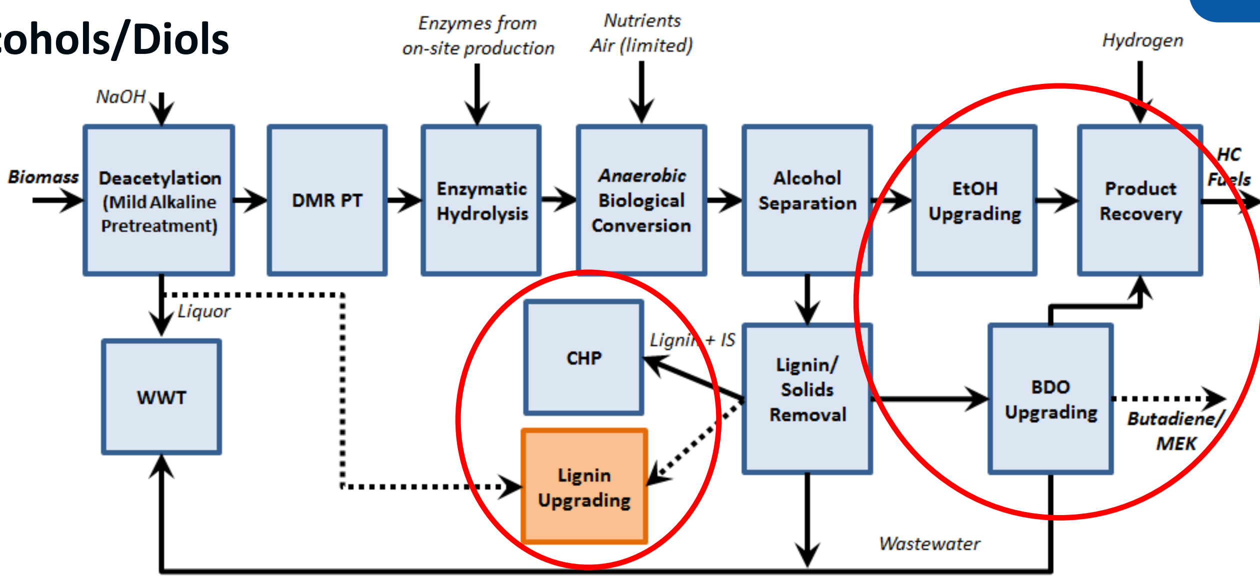
(BUS)



Anaerobic pathways:
Lower fermentation costs, more-complex upgrading (short-chain oxygenates)

Mixed Alcohols/Diols

(TMD, BSI)



Prior TEA for $3/GGE Goals: Key Inputs for Pathways

Lipids

Lipid Pathway: Parameter	*Projection*
Lipid productivity (g/L-hr)	1.0
Lipid content (wt%)	70%
Conversion: Glucose → Lipid [total utilization] (%)	82% [100%]
Conversion: Xylose → Lipid [total utilization] (%)	81% [85%]
Conversion: Arabinose → Lipid [total utilization] (%)	81% [85%]
Modeled metabolic yield [Process yield] (g/g sugar)	0.27 [0.25]
Product recovery method	Autolyse
Product recovery yield	95%
Upgrading yield to fuels (wt% of lipid feed)	81 wt%
C yield across upgrading (C in fuel product/C in feed)	89%

Acids

Organic Acids Pathway: Parameter	*Projection*
Fermentation residence time (days)	1.5
Glucose utilization (%)	95%
Xylose utilization (%)	85%
Arabinose utilization (%)	85%
Modeled metabolic yield [Process yield] (g/g sugar)	0.41 [0.39]
Product recovery method	Low-pH pertractive fermentation
Product recovery yield	>99%
Upgrading yield to fuels (wt% of organic acid intermediate)	66 wt%
C yield across upgrading (C in fuel product/ C in acid)	89%

Fatty Alcohols

Fatty Alcohol Pathway: Parameter	*Projection*
FaOH productivity (g/L-hr)	1.0
FaOH theoretical metabolic yield (g/g sugar consumed)	0.28
FaOH modeled metabolic yield (g/g sugar consumed)	0.252
Conversion: Glucose → FaOH [total utilization] (%)	90% [100%]
Conversion: Xylose → FaOH [total utilization] (%)	90% [85%]
Conversion: Arabinose → FaOH [total utilization] (%)	90% [85%]
Product recovery method	Overlay-assisted secretion
Overlay:Broth Volume	1:10
Product recovery yield	95%
Upgrading yield to fuels (wt% of FaOH feed)	92 wt%
C yield across upgrading (C in fuel product/ C in feed)	98.5%

Alcohols/Diols

Alcohols/Diols Pathway: Parameter	*Projection*
Fermentation batch time (days)	1.5
Conversion: Glucose → 2,3-BDO [total utilization] (%)	85% [95%]
Conversion: Xylose → 2,3-BDO [total utilization] (%)	70% [85%]
Conversion: Arabinose → 2,3-BDO [total utilization] (%)	0% [85%]
Conversion: Glucose → Ethanol [total utilization] (%)	10% [95%]
Conversion: Xylose → Ethanol [total utilization] (%)	15% [85%]
Conversion: Arabinose → Ethanol [total utilization] (%)	85% [88%]
Modeled metabolic yield [Process yield] (g/g sugar)	0.51 [0.49]
Product recovery method	Distillation
Ethanol recovery yield	98%
2,3-BDO recovery yield	96%
C yield across upgrading (C in fuel product/C in feed)	91%

Historical Progress on Lipid Pathway SOT Performance

Lipids Pathway	FY13	FY14	FY15	FY16	FY17	Final Target
Fermentation basis	varies	SS/B	SS/FB	WS/FB	WS/FB	WS/FB
Lipid productivity (g/L-hr)	0.11-0.21	0.29	0.34	0.68	0.97	1.0
Lipid content (cell wt%)	34%	57%	60%	62%	68%	70%
Glucose conversion to product (%)	52%	75%	75%	78%	79%	82%
Xylose conversion to product (%)	35%	74%	44%	77%	77%	69%
Arabinose conversion to product (%)	0-3%	0%	0%	0%	0%	69%
Process yield (g/g sugars)	0.15	0.26	0.24	0.24	0.26	0.25
Lipid recovery (method)	90% (extract)	90% (extract)	90% (extract)	90% (extract)	90% (extract)	95% (autolyse)
Lipid upgrading: final fuel yield (C%)	88%	88%	88%	88%	88%	88%

- Significant historical progress made on lipid yeast pathway over short timeframe (5 years), including 5X improvement in productivity, 2X improvement in lipid content, and 1.7X improvement in overall fermentation process yield – latest data near final targets
- BUT, key challenge remains to achieve cell autolysis for lipid recovery (avoid extraction) – significant R&D barrier to overcome through strain engineering
- Even if autolysis could be achieved, target case would still be ~$2/GGE higher than anaerobic options